# New mono- and di-nuclear complexes of PdII, PtII and NiII of PNNP ligands with a 2,2'-biaryl bridging unit

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# 3 CIF's belonging to 7/04170E     (From A.L.Spek - Utrecht University)

# ***** Complex 1 *******

# CIF-file generated for  (C26H22ClNPPd)2               CP339

#======================================================================

data_cp339

#======================================================================

# 5. CHEMICAL DATA

_chemical_name_systematic
;
 ?
;
_chemical_name_common            ?
_chemical_melting_point          ?
_chemical_formula_moiety         'C52 H44 Cl2 N2 P2 Pd2'
_chemical_formula_structural     ?
_chemical_formula_sum           'C52 H44 Cl2 N2 P2 Pd2'
_chemical_formula_weight          1042.63
_chemical_compound_source        ?

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
Pd  Pd    -.9988    1.0072
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 P   P     .1023     .0942
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 N   N     .0061     .0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cl  Cl     .1484     .1585
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 H   H     .0000     .0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 C   C     .0033     .0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#======================================================================

# 6. CRYSTAL DATA

_symmetry_cell_setting             Monoclinic
_symmetry_space_group_name_H-M   'C 2/c'

loop_
_symmetry_equiv_pos_as_xyz
 x,y,z
 -x,y,1/2-z
 -x,-y,-z
 x,-y,1/2+z
 1/2+x,1/2+y,z
 1/2-x,1/2+y,1/2-z
 1/2-x,1/2-y,-z
 1/2+x,1/2-y,1/2+z

```
_cell_length_a                      17.789(5)
_cell_length_b                      14.170(4)
_cell_length_c                      19.423(7)
_cell_angle_alpha                          90
_cell_angle_beta                    113.02(2)
_cell_angle_gamma                          90
_cell_volume                          4506(3)
_cell_formula_units_Z               4
_cell_measurement_temperature       130(2)
_cell_measurement_reflns_used    22
_cell_measurement_theta_min      18.00
_cell_measurement_theta_max      20.47
_cell_special_details
; ?
;

_exptl_crystal_description       'irregular fragment'
_exptl_crystal_colour            orange
_exptl_crystal_size_max          0.50
_exptl_crystal_size_mid          0.44
_exptl_crystal_size_min          0.19
_exptl_crystal_size_rad          ?
_exptl_crystal_density_meas     'Not Measured'
_exptl_crystal_density_diffrn    1.537
_exptl_crystal_density_method    ?
_exptl_crystal_F_000             2104
_exptl_absorpt_coefficient_mu    1.03
_exptl_crystal_density_meas_temp ?
_exptl_absorpt_correction_type   ?
_exptl_absorpt_correction_T_min  ?
_exptl_absorpt_correction_T_max  ?

#=============================================================

# 7. EXPERIMENTAL DATA

_exptl_special_details
; ?
;
_diffrn_ambient_temperature      130(2)
_diffrn_radiation_wavelength     71073
_diffrn_radiation_type           'Mo K\a'

_diffrn_radiation_source         'fine-focus sealed tube'
_diffrn_radiation_monochromator  graphite



_diffrn_measurement_device_type  CAD4F
_diffrn_measurement_method       '\w/2\q scan'

_diffrn_special_details
;
 Crystal into the cold nitrogen stream  of the low-temperature
unit
 (Bolhuis, 1971), on an Enraf-Nonius CAD4-4F diffractometer.
   Graphite-monochromated Mo K\a radiation,
 \w/2\q scan, \D\w = (1.00 + 0.34 tg \q)\%.
;

_diffrn_standards_number         3
_diffrn_standards_interval_count ?'
_diffrn_standards_interval_time  10800
_diffrn_standards_decay_%        .7?

loop_
_diffrn_standard_refln_index_h
```

```
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
  -1 -3  0
  -2  2 -2
   1  3 -4
# number of measured reflections (redundant set)
_diffrn_reflns_number           9610
_diffrn_reflns_av_R_equivalents ?
_diffrn_reflns_av_sigmaI/netI   0.036
_diffrn_reflns_limit_h_min      -22
_diffrn_reflns_limit_h_max      22
_diffrn_reflns_limit_k_min      -17
_diffrn_reflns_limit_k_max      16
_diffrn_reflns_limit_l_min      -24
_diffrn_reflns_limit_l_max      13
_diffrn_reflns_theta_min        1.14
_diffrn_reflns_theta_max        26.5
_diffrn_reflns_reduction_process
;
 Intensity data were corrected for Lorentz and polarization
effects, scale
 variation, but not for absorption and reduced to F~o~^2^
;

# number of unique reflections
_reflns_number_total            4678
# number of observed reflections (> n sig(I))
_reflns_number_gt               ?
_reflns_threshold_expression     >0

_computing_data_collection       ?
_computing_cell_refinement       ?
_computing_data_reduction        ?
_computing_structure_solution     'DIRDIF4 (Beurskens, 1994)'
_computing_structure_refinement   'SHELXL-93 (Sheldrick, 1993)'
_computing_molecular_graphics    ?
_computing_publication_material  'PLATON (Spek, 1990)'

#=============================================================

# 8. REFINEMENT DATA

_refine_special_details          ?
_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme
 'calc w=1/[\s^2^(Fo^2^)+(0.06622P)^2^+28.60P] where P=(Fo^2^+2Fc^2^)/3'
_refine_ls_hydrogen_treatment    'isotropic refinement '
_refine_ls_extinction_method      ?
_refine_ls_extinction_coef       ?
_refine_ls_extinction_expression ?
_refine_ls_abs_structure_details
;
 ?
;
_refine_ls_abs_structure_Flack   ?
_refine_ls_number_reflns         4269
_refine_ls_number_parameters     359
_refine_ls_number_restraints      ?
_refine_ls_number_constraints    ?
_refine_ls_R_factor_all          ?
_refine_ls_R_factor_gt           0.0471
_refine_ls_wR_factor_obs         .1298
_refine_ls_wR_factor_ref         ?
_refine_ls_goodness_of_fit_ref    1.083
_refine_ls_restrained_S_all      ?
_refine_ls_restrained_S_obs      ?
```

```
_refine_ls_shift/su_max          ?
_refine_ls_shift/esd_mean        '< 0.001'
_refine_diff_density_max         1.22(13)
_refine_diff_density_min         -1.14

#=============================================================

# 9. ATOMIC COORDINATES AND THERMAL PARAMETERS

loop_
_atom_site_label
_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
 Pd      Uani     .05929(2)    .27636(2)    .09370(2)     1.000
.0279(1)
 Cl      Uani    -.07207(6)    .20936(7)    .03460(6)     1.000
.0306(3)
 P       Uani     .18205(7)    .33582(9)    .15168(7)     1.000
.0326(4)
 N       Uani      .0878(2)     .2244(3)     .2100(2)     1.000
.0267(11)
 C1      Uani      .2635(3)     .2536(4)     .1610(3)     1.000
.0370(14)
 C2      Uani      .2604(4)     .2023(5)     .0996(4)     1.000
.0489(19)
 C3      Uani      .3215(5)     .1408(5)     .1045(5)     1.000
 .062(3)
 C4      Uani      .3866(4)     .1275(5)     .1717(5)     1.000
 .062(2)
 C5      Uani      .3899(4)     .1773(5)     .2341(5)     1.000
 .060(2)
 C6      Uani      .3284(3)     .2401(4)     .2271(4)     1.000
.0432(17)
 C7      Uani      .2145(3)     .4466(4)     .1255(3)     1.000
.0369(16)
 C8      Uani      .1686(4)     .5264(4)     .1215(4)     1.000
.0495(19)
 C9      Uani      .1914(4)     .6115(4)     .0997(4)     1.000
 .054(2)
 C10     Uani      .2564(3)     .6158(4)     .0792(3)     1.000
.0462(17)
 C11     Uani      .3006(3)     .5370(4)     .0806(3)     1.000
.0460(17)
 C12     Uani      .2810(3)     .4511(4)     .1048(3)     1.000
.0383(16)
 C13     Uani      .1842(3)     .3535(3)     .2443(3)     1.000
.0315(12)
 C14     Uani      .2339(3)     .4164(4)     .2968(3)     1.000
.0403(17)
 C15     Uani      .2282(3)     .4257(4)     .3651(3)     1.000
.0426(17)
 C16     Uani      .1704(3)     .3748(4)     .3802(3)     1.000
.0407(17)
 C17     Uani      .1217(3)     .3104(3)     .3299(3)     1.000
.0346(16)
 C18     Uani      .1298(3)     .2965(3)     .2624(3)     1.000
.0281(12)
 C19     Uani      .0768(3)     .1452(3)     .2372(3)     1.000
.0254(12)
 C20     Uani      .0481(3)     .0599(3)     .1930(3)     1.000
.0267(12)
 C21     Uani      .0678(3)     .0468(3)     .1306(3)     1.000
.0325(14)
```

```
 C22     Uani      .0501(3)    -.0358(4)     .0904(3)     1.000
.0374(16)
 C23     Uani      .0099(3)    -.1065(4)     .1110(3)     1.000
.0420(16)
 C24     Uani     -.0098(3)    -.0952(3)     .1731(3)     1.000
.0362(16)
 C25     Uani      .0093(3)    -.0133(3)     .2159(2)     1.000
.0258(11)
 C26     Uani      .0444(4)     .3446(5)    -.0021(3)     1.000
 .048(2)
 H2      Uiso       .217(4)      .205(4)      .062(4)     1.000
.043(17)
 H3      Uiso       .322(4)      .100(5)      .066(4)     1.000
  .06(2)
 H4      Uiso       .428(4)      .088(5)      .178(4)     1.000
.060(19)
 H5      Uiso       .438(4)      .164(4)      .281(4)     1.000
.039(15)
 H6      Uiso       .335(4)      .260(4)      .264(4)     1.000
.034(16)
 H8      Uiso       .124(4)      .517(4)      .139(4)     1.000
.051(17)
 H9      Uiso       .161(3)      .655(4)      .096(3)     1.000
.028(14)
 H10     Uiso       .269(3)      .669(4)      .063(3)     1.000
.036(14)
 H11     Uiso       .344(4)      .543(5)      .067(4)     1.000
.058(19)
 H12     Uiso       .318(3)      .402(4)      .112(3)     1.000
.021(11)
 H14     Uiso       .272(4)      .453(5)      .287(4)     1.000
  .07(2)
 H15     Uiso       .260(4)      .461(4)      .391(4)     1.000
.043(16)
 H16     Uiso       .163(3)      .389(4)      .426(3)     1.000
.041(15)
 H17     Uiso       .090(3)      .278(4)      .345(3)     1.000
.034(14)
 H19     Uiso       .087(3)      .141(3)      .279(3)     1.000
.015(11)
 H21     Uiso       .089(3)      .088(4)      .114(3)     1.000
.033(14)
 H22     Uiso       .061(3)     -.042(4)      .044(3)     1.000
.037(14)
 H23     Uiso      -.004(4)     -.156(5)      .084(4)     1.000
.049(17)
 H24     Uiso      -.035(3)     -.144(4)      .190(3)     1.000
.037(14)
 H26     Uiso       .036(6)      .398(8)      .008(6)     1.000
  .11(4)
 H26'    Uiso      -.002(5)      .330(6)     -.040(5)     1.000
  .07(2)
 H26"    Uiso       .083(5)      .321(6)     -.016(5)     1.000
  .08(2)

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
  Pd        .0312(2)   .0289(2)   .0273(2)   -.0004(1)
.0155(2)   -.0088(1)
  Cl        .0307(5)   .0289(5)   .0358(6)   -.0049(4)
.0170(4)   -.0060(4)
```

```
  P          .0335(6)   .0333(6)   .0353(7)   -.0002(5)
.0182(5)   -.0109(5)
  N         .0304(18)  .0261(18)  .0274(19)  -.0017(15)
.0154(15)  -.0045(14)
  C1          .037(2)    .036(2)    .046(3)     .002(2)
.025(2)    -.010(2)
  C2          .052(3)    .051(3)    .051(4)    -.004(3)
.028(3)    -.009(3)
  C3          .071(4)    .051(4)    .090(5)    -.016(4)
.059(4)    -.012(3)
  C4          .043(3)    .049(3)    .108(6)    -.004(4)
.044(4)    -.002(3)
  C5          .043(3)    .053(4)    .089(5)     .005(4)
.030(4)    -.001(3)
  C6          .036(3)    .050(3)    .047(3)     .002(3)
.020(3)     .000(2)
  C7          .036(2)    .038(3)    .038(3)     .004(2)
.016(2)    -.013(2)
  C8          .047(3)    .042(3)    .065(4)     .007(3)
.028(3)    -.008(2)
  C9          .058(4)    .036(3)    .065(4)     .007(3)
.021(3)    -.008(3)
  C10         .048(3)    .045(3)    .036(3)     .009(2)
.006(2)    -.027(3)
  C11         .040(3)    .054(3)    .043(3)     .007(3)
.015(2)    -.025(3)
  C12         .034(2)    .044(3)    .037(3)     .007(2)
.014(2)    -.011(2)
  C13         .032(2)    .033(2)    .030(2)  -.0001(19)
.0128(19)  -.0066(18)
  C14         .039(3)    .038(3)    .043(3)    -.006(2)
.015(2)    -.013(2)
  C15         .045(3)    .038(3)    .039(3)    -.012(2)
.010(2)    -.011(2)
  C16         .055(3)    .038(3)    .032(3)    -.004(2)
.020(2)    -.003(2)
  C17         .046(3)    .031(2)    .033(3)  -.0008(19)
.022(2)    -.005(2)
  C18         .031(2)    .028(2)    .027(2)  -.0011(18)
.0133(18)  -.0068(18)
  C19         .026(2)    .030(2)    .024(2)   .0041(18)
.0140(17)   .0017(17)
  C20         .026(2)    .025(2)    .029(2)   .0045(17)
.0108(17)   .0070(16)
  C21         .034(2)    .031(2)    .034(3)     .005(2)
.015(2)   .0057(19)
  C22         .044(3)    .042(3)    .028(2)    -.003(2)
.016(2)     .013(2)
  C23         .055(3)    .029(2)    .042(3)    -.013(2)
.019(2)     .003(2)
  C24         .041(3)    .025(2)    .043(3)    -.004(2)
.017(2)  -.0007(19)
  C25         .028(2)  .0206(19)    .029(2)   .0009(17)
.0115(18)   .0029(16)
  C26         .055(4)    .057(4)    .031(3)     .008(3)
.016(3)    -.023(3)

#===============================================================

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
 Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All esds are estimated
 from the variances of the (full) variance-covariance matrix.
 The cell esds are taken into account in the estimation of
```

```
 distances, angles and torsion angles
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 Pd      Cl      2.3625(15)                    .       .
          yes
 Pd      P       2.1963(16)                    .       .
          yes
 Pd      N         2.237(4)                    .       .
          yes
 Pd      C26       2.020(6)                    .       .
          yes
 P       C1        1.812(6)                    .       .
          yes
 P       C7        1.813(6)                    .       .
          yes
 P       C13       1.802(6)                    .       .
          yes
 N       C18       1.429(6)                    .       .
          yes
 N       C19       1.288(6)                    .       .
          yes
 C1      C2        1.379(9)                    .       .
          no
 C1      C6        1.363(9)                    .       .
          no
 C2      C3       1.367(11)                    .       .
          no
 C3      C4       1.378(13)                    .       .
          no
 C4      C5       1.384(12)                    .       .
          no
 C5      C6       1.375(10)                    .       .
          no
 C7      C8        1.379(9)                    .       .
          no
 C7      C12       1.392(8)                    .       .
          no
 C8      C9        1.390(9)                    .       .
          no
 C9      C10      1.364(10)                    .       .
          no
 C10     C11       1.360(8)                    .       .
          no
 C11     C12       1.397(8)                    .       .
          no
 C13     C14       1.382(7)                    .       .
          no
 C13     C18       1.407(8)                    .       .
          no
 C14     C15       1.376(8)                    .       .
          no
 C15     C16       1.378(8)                    .       .
          no
 C16     C17       1.370(7)                    .       .
          no
 C17     C18       1.388(8)                    .       .
          no
 C19     C20       1.455(7)                    .       .
          no
 C20     C21       1.399(8)                    .       .
```

```
          no
 C20      C25        1.411(7)                    .       .
          no
 C21      C22        1.373(7)                    .       .
          no
 C22      C23        1.378(8)                    .       .
          no
 C23      C24        1.391(8)                    .       .
          no
 C24      C25        1.390(6)                    .       .
          no
 C25      C25        1.486(6)                    .     2_555
          no
 C2       H2           .83(7)                    .       .
          no
 C3       H3           .95(7)                    .       .
          no
 C4       H4           .89(8)                    .       .
          no
 C5       H5           .99(7)                    .       .
          no
 C6       H6           .74(7)                    .       .
          no
 C8       H8           .99(8)                    .       .
          no
 C9       H9           .80(6)                    .       .
          no
 C10      H10          .88(6)                    .       .
          no
 C11      H11          .91(8)                    .       .
          no
 C12      H12          .93(6)                    .       .
          no
 C14      H14          .93(8)                    .       .
          no
 C15      H15          .78(7)                    .       .
          no
 C16      H16          .97(6)                    .       .
          no
 C17      H17          .86(6)                    .       .
          no
 C19      H19          .76(5)                    .       .
          no
 C21      H21          .83(6)                    .       .
          no
 C22      H22         1.00(6)                    .       .
          no
 C23      H23          .85(7)                    .       .
          no
 C24      H24          .95(6)                    .       .
          no
 C26      H26         .81(11)                    .       .
          no
 C26      H26'         .89(9)                    .       .
          no
 C26      H26"         .90(9)                    .       .
          no

loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
```

```
 Cl      Pd      P         178.21(5)            .       .
.           yes
 Cl      Pd      N         98.57(11)            .       .
.           yes
 Cl      Pd      C26         89.8(2)            .       .
.           yes
 P       Pd      N         79.70(11)            .       .
.           yes
 P       Pd      C26         92.0(2)            .       .
.           yes
 N       Pd      C26        169.6(2)            .       .
.           yes
 Pd      P       C1       113.60(19)            .       .
.           yes
 Pd      P       C7       123.39(19)            .       .
.           yes
 Pd      P       C13      101.18(19)            .       .
.           yes
 C1      P       C7          104.8(3)           .       .
.           yes
 C1      P       C13         106.6(2)           .       .
.           yes
 C7      P       C13         106.0(2)           .       .
.           yes
 Pd      N       C18         109.4(3)           .       .
.           yes
 Pd      N       C19         133.7(3)           .       .
.           yes
 C18     N       C19         116.9(4)           .       .
.           yes
 P       C1      C2          119.5(5)           .       .
.           yes
 P       C1      C6          122.3(4)           .       .
.           yes
 C2      C1      C6          118.2(6)           .       .
.           no
 C1      C2      C3          120.9(7)           .       .
.           no
 C2      C3      C4          120.3(8)           .       .
.           no
 C3      C4      C5          119.5(7)           .       .
.           no
 C4      C5      C6          118.9(8)           .       .
.           no
 C1      C6      C5          122.1(7)           .       .
.           no
 P       C7      C8          118.6(5)           .       .
.           yes
 P       C7      C12         121.4(4)           .       .
.           yes
 C8      C7      C12         119.8(6)           .       .
.           no
 C7      C8      C9          119.4(7)           .       .
.           no
 C8      C9      C10         120.6(6)           .       .
.           no
 C9      C10     C11         120.5(5)           .       .
.           no
 C10     C11     C12         120.2(5)           .       .
.           no
 C7      C12     C11         119.3(5)           .       .
.           no
 P       C13     C14         125.7(4)           .       .
.           yes
 P       C13     C18         114.9(4)           .       .
.           yes
 C14     C13     C18         119.3(5)           .       .
```

```
.           no
 C13     C14     C15        120.4(5)            .       .
.           no
 C14     C15     C16        119.8(5)            .       .
.           no
 C15     C16     C17        120.9(5)            .       .
.           no
 C16     C17     C18        119.9(5)            .       .
.           no
 N       C18     C13        116.8(5)            .       .
.           yes
 N       C18     C17        123.8(5)            .       .
.           yes
 C13     C18     C17        119.4(5)            .       .
.           no
 N       C19     C20        123.8(5)            .       .
.           yes
 C19     C20     C21        118.2(5)            .       .
.           no
 C19     C20     C25        121.8(5)            .       .
.           no
 C21     C20     C25        119.6(4)            .       .
.           no
 C20     C21     C22        121.7(5)            .       .
.           no
 C21     C22     C23        119.0(5)            .       .
.           no
 C22     C23     C24        120.2(5)            .       .
.           no
 C23     C24     C25        122.0(5)            .       .
.           no
 C20     C25     C24        117.4(4)            .       .
.           no
 C20     C25     C25        126.0(4)            .       .
2_555         no
 C24     C25     C25        116.5(4)            .       .
2_555         no
 C1      C2      H2           116(5)            .       .
.           no
 C3      C2      H2           122(5)            .       .
.           no
 C2      C3      H3           126(5)            .       .
.           no
 C4      C3      H3           114(5)            .       .
.           no
 C3      C4      H4           124(5)            .       .
.           no
 C5      C4      H4           117(5)            .       .
.           no
 C4      C5      H5           116(4)            .       .
.           no
 C6      C5      H5           125(4)            .       .
.           no
 C1      C6      H6           128(6)            .       .
.           no
 C5      C6      H6           110(6)            .       .
.           no
 C7      C8      H8           114(3)            .       .
.           no
 C9      C8      H8           126(3)            .       .
.           no
 C8      C9      H9           115(4)            .       .
.           no
 C10     C9      H9           124(4)            .       .
.           no
 C9      C10     H10          120(4)            .       .
.           no
```

```
 C11     C10     H10          119(4)              .       .
.           no
 C10     C11     H11          118(5)              .       .
.           no
 C12     C11     H11          122(5)              .       .
.           no
 C7      C12     H12          124(4)              .       .
.           no
 C11     C12     H12          117(4)              .       .
.           no
 C13     C14     H14          121(4)              .       .
.           no
 C15     C14     H14          119(4)              .       .
.           no
 C14     C15     H15          112(6)              .       .
.           no
 C16     C15     H15          128(6)              .       .
.           no
 C15     C16     H16          118(3)              .       .
.           no
 C17     C16     H16          121(3)              .       .
.           no
 C16     C17     H17          115(4)              .       .
.           no
 C18     C17     H17          125(4)              .       .
.           no
 N       C19     H19          120(3)              .       .
.           no
 C20     C19     H19          117(3)              .       .
.           no
 C20     C21     H21          123(4)              .       .
.           no
 C22     C21     H21          115(4)              .       .
.           no
 C21     C22     H22          120(3)              .       .
.           no
 C23     C22     H22          120(3)              .       .
.           no
 C22     C23     H23          119(5)              .       .
.           no
 C24     C23     H23          121(5)              .       .
.           no
 C23     C24     H24          122(3)              .       .
.           no
 C25     C24     H24          116(3)              .       .
.           no
 Pd      C26     H26          101(8)              .       .
.           no
 Pd      C26     H26'         113(6)              .       .
.           no
 Pd      C26     H26"         105(6)              .       .
.           no
 H26     C26     H26'        103(10)              .       .
.           no
 H26     C26     H26"        131(10)              .       .
.           no
 H26'    C26     H26"         104(8)              .       .
.           no

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 N       Pd      P       C1          83.8(2)     .       .
.       .   no
 N       Pd      P       C7        -147.8(3)     .       .
.       .   no
 N       Pd      P       C13      -30.05(19)     .       .
.       .   no
 C26     Pd      P       C1        -102.5(3)     .       .
.       .   no
 C26     Pd      P       C7          25.9(3)     .       .
.       .   no
 C26     Pd      P       C13        143.7(3)     .       .
.       .   no
 Cl      Pd      N       C18       -141.1(3)     .       .
.       .   no
 Cl      Pd      N       C19         41.7(5)     .       .
.       .   no
 P       Pd      N       C18         39.3(3)     .       .
.       .   no
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.       .   no
 Pd      P       C1      C2          47.6(6)     .       .
.       .   no
 Pd      P       C1      C6        -132.3(5)     .       .
.       .   no
 C7      P       C1      C2         -89.9(5)     .       .
.       .   no
 C7      P       C1      C6          90.3(5)     .       .
.       .   no
 C13     P       C1      C2         158.1(5)     .       .
.       .   no
 C13     P       C1      C6         -21.7(6)     .       .
.       .   no
 Pd      P       C7      C8          54.4(5)     .       .
.       .   no
 Pd      P       C7      C12       -121.3(4)     .       .
.       .   no
 C1      P       C7      C8        -173.5(5)     .       .
.       .   no
 C1      P       C7      C12         10.8(5)     .       .
.       .   no
 C13     P       C7      C8         -61.0(5)     .       .
.       .   no
 C13     P       C7      C12        123.3(5)     .       .
.       .   no
 Pd      P       C13     C14       -157.0(5)     .       .
.       .   no
 Pd      P       C13     C18         23.3(4)     .       .
.       .   no
 C1      P       C13     C14         84.0(5)     .       .
.       .   no
 C1      P       C13     C18        -95.7(4)     .       .
.       .   no
 C7      P       C13     C14        -27.2(6)     .       .
.       .   no
 C7      P       C13     C18        153.1(4)     .       .
.       .   no
 Pd      N       C18     C13        -35.5(5)     .       .
.       .   no
 Pd      N       C18     C17        146.8(4)     .       .
.       .   no
 C19     N       C18     C13        142.2(5)     .       .
.       .   no
 C19     N       C18     C17        -35.5(7)     .       .
.       .   no
```

| | | | | | | |
|---|---|---|---|---|---|---|
| Pd | N | C19 | C20 | 7.9(8) | . | . |
| . | . | no | | | | |
| C18 | N | C19 | C20 | -169.1(5) | . | . |
| . | . | no | | | | |
| P | C1 | C2 | C3 | 179.0(6) | . | . |
| . | . | no | | | | |
| C6 | C1 | C2 | C3 | -1.2(10) | . | . |
| . | . | no | | | | |
| P | C1 | C6 | C5 | 179.7(6) | . | . |
| . | . | no | | | | |
| C2 | C1 | C6 | C5 | -.2(10) | . | . |
| . | . | no | | | | |
| C1 | C2 | C3 | C4 | 1.5(12) | . | . |
| . | . | no | | | | |
| C2 | C3 | C4 | C5 | -.4(12) | . | . |
| . | . | no | | | | |
| C3 | C4 | C5 | C6 | -.9(11) | . | . |
| . | . | no | | | | |
| C4 | C5 | C6 | C1 | 1.3(10) | . | . |
| . | . | no | | | | |
| P | C7 | C8 | C9 | -178.4(5) | . | . |
| . | . | no | | | | |
| C12 | C7 | C8 | C9 | -2.6(9) | . | . |
| . | . | no | | | | |
| P | C7 | C12 | C11 | 176.0(4) | . | . |
| . | . | no | | | | |
| C8 | C7 | C12 | C11 | .4(8) | . | . |
| . | . | no | | | | |
| C7 | C8 | C9 | C10 | 2.9(10) | . | . |
| . | . | no | | | | |
| C8 | C9 | C10 | C11 | -.8(10) | . | . |
| . | . | no | | | | |
| C9 | C10 | C11 | C12 | -1.5(9) | . | . |
| . | . | no | | | | |
| C10 | C11 | C12 | C7 | 1.7(8) | . | . |
| . | . | no | | | | |
| P | C13 | C14 | C15 | 178.0(4) | . | . |
| . | . | no | | | | |
| C18 | C13 | C14 | C15 | -2.3(8) | . | . |
| . | . | no | | | | |
| P | C13 | C18 | N | 7.7(6) | . | . |
| . | . | no | | | | |
| P | C13 | C18 | C17 | -174.5(4) | . | . |
| . | . | no | | | | |
| C14 | C13 | C18 | N | -172.0(5) | . | . |
| . | . | no | | | | |
| C14 | C13 | C18 | C17 | 5.8(8) | . | . |
| . | . | no | | | | |
| C13 | C14 | C15 | C16 | -2.6(9) | . | . |
| . | . | no | | | | |
| C14 | C15 | C16 | C17 | 4.1(9) | . | . |
| . | . | no | | | | |
| C15 | C16 | C17 | C18 | -.6(8) | . | . |
| . | . | no | | | | |
| C16 | C17 | C18 | N | 173.3(5) | . | . |
| . | . | no | | | | |
| C16 | C17 | C18 | C13 | -4.3(8) | . | . |
| . | . | no | | | | |
| N | C19 | C20 | C21 | 30.3(8) | . | . |
| . | . | no | | | | |
| N | C19 | C20 | C25 | -156.7(5) | . | . |
| . | . | no | | | | |
| C19 | C20 | C21 | C22 | 173.4(5) | . | . |
| . | . | no | | | | |
| C25 | C20 | C21 | C22 | .2(8) | . | . |
| . | . | no | | | | |
| C19 | C20 | C25 | C24 | -174.8(5) | . | . |

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 C19     C20     C25     C25          1.7(8)     .       .
.     2_555 no
 C21     C20     C25     C24         -1.8(8)     .       .
.       .   no
 C21     C20     C25     C25        174.7(5)     .       .
.     2_555 no
 C20     C21     C22     C23          1.8(8)     .       .
.       .   no
 C21     C22     C23     C24         -2.2(8)     .       .
.       .   no
 C22     C23     C24     C25           .5(8)     .       .
.       .   no
 C23     C24     C25     C20          1.5(8)     .       .
.       .   no
 C23     C24     C25     C25       -175.4(5)     .       .
.     2_555 no
 C20     C25     C25     C20         49.2(8)     .       .
2_555   2_555 no
 C20     C25     C25     C24       -134.2(5)     .       .
2_555   2_555 no
 C24     C25     C25     C20       -134.2(5)     .       .
2_555   2_555 no
 C24     C25     C25     C24         42.3(7)     .       .
2_555   2_555 no

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 Pd      C21        3.322(4)                    .       .
          no
 Pd      C17        4.067(6)                    .     2_555
          no
 Cl      C22        3.583(6)                    .     3_555
          no
 Cl      C17        3.402(6)                    .     2_555
          no
 Cl      C21        3.368(5)                    .       .
          no
 C2      C12        3.542(9)                    .       .
          no
 C3      C15        3.291(9)                    .     6_545
          no
 C4      C15        3.423(9)                    .     6_545
          no
 C6      C14        3.561(8)                    .       .
          no
 C8      C14        3.504(9)                    .       .
          no
 C10     C16        3.560(8)                    .     4_564
          no
 C10     C17        3.525(8)                    .     6_555
          no
 C12     C24        3.490(8)                    .     5_555
          no
 C12     C2         3.542(9)                    .       .
          no
 C14     C8         3.504(9)                    .       .
          no
 C14     C6         3.561(8)                    .       .
          no
 C15     C3         3.291(9)                    .     6_555
          no
```

| | | | | |
|---|---|---|---|---|
| C15 | C4 | 3.423(9) | . | 6_555 |
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| C16 | C10 | 3.560(8) | . | 4_565 |
| | no | | | |
| C17 | C10 | 3.525(8) | . | 6_545 |
| | no | | | |
| C17 | Cl | 3.402(6) | . | 2_555 |
| | no | | | |
| C17 | Pd | 4.067(6) | . | 2_555 |
| | no | | | |
| C19 | C20 | 3.254(8) | . | 2_555 |
| | no | | | |
| C19 | C19 | 2.962(8) | . | 2_555 |
| | no | | | |
| C20 | C19 | 3.254(8) | . | 2_555 |
| | no | | | |
| C21 | Pd | 3.322(4) | . | . |
| | no | | | |
| C21 | Cl | 3.368(5) | . | . |
| | no | | | |
| C22 | Cl | 3.583(6) | . | 3_555 |
| | no | | | |
| C22 | C22 | 3.412(8) | . | 3_555 |
| | no | | | |
| C24 | C12 | 3.490(8) | . | 5_445 |
| | no | | | |
| Pd | H17 | 3.31(6) | . | 2_555 |
| | no | | | |
| Pd | H8 | 3.60(6) | . | . |
| | no | | | |
| Pd | H23 | 3.62(7) | . | 3_555 |
| | no | | | |
| Pd | H2 | 3.26(8) | . | . |
| | no | | | |
| Pd | H21 | 2.72(6) | . | . |
| | no | | | |
| Cl | H22 | 2.87(6) | . | 3_555 |
| | no | | | |
| Cl | H11 | 2.99(7) | . | 5_445 |
| | no | | | |
| Cl | H10 | 3.14(6) | . | 5_445 |
| | no | | | |
| Cl | H9 | 3.08(6) | . | 3_565 |
| | no | | | |
| Cl | H17 | 2.66(6) | . | 2_555 |
| | no | | | |
| N | H21 | 2.69(6) | . | . |
| | no | | | |
| C1 | H12 | 2.64(6) | . | . |
| | no | | | |
| C2 | H12 | 2.99(6) | . | . |
| | no | | | |
| C3 | H26" | 2.90(9) | . | 7_555 |
| | no | | | |
| C3 | H15 | 2.95(6) | . | 6_545 |
| | no | | | |
| C4 | H5 | 2.93(8) | . | 2_655 |
| | no | | | |
| C7 | H14 | 2.90(7) | . | . |
| | no | | | |
| C10 | H16 | 2.78(5) | . | 4_564 |
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| C10 | H19 | 3.08(6) | . | 6_555 |
| | no | | | |
| C11 | H19 | 3.06(5) | . | 6_555 |
| | no | | | |
| C13 | H8 | 3.00(6) | . | . |

| | | | | |
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| | no | | | |
| C13 | H6 | 2.88(7) | . | . |
| | no | | | |
| C14 | H6 | 3.07(7) | . | . |
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| C17 | H19 | 2.58(4) | . | . |
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| C19 | H17 | 2.76(6) | . | . |
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| C19 | H19 | 2.81(6) | . | 2_555 |
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| C20 | H19 | 2.90(6) | . | 2_555 |
| | no | | | |
| C21 | H14 | 2.98(7) | . | 6_545 |
| | no | | | |
| C22 | H22 | 2.81(5) | . | 3_555 |
| | no | | | |
| C24 | H24 | 2.55(5) | . | 2_555 |
| | no | | | |
| C24 | H12 | 2.82(6) | . | 5_445 |
| | no | | | |
| C25 | H19 | 2.80(5) | . | 2_555 |
| | no | | | |
| C26 | H23 | 3.05(7) | . | 3_555 |
| | no | | | |
| H2 | Pd | 3.26(8) | . | . |
| | no | | | |
| H3 | H26" | 2.52(12) | . | 7_555 |
| | no | | | |
| H4 | H5 | 2.45(11) | . | 2_655 |
| | no | | | |
| H5 | C4 | 2.93(8) | . | 2_655 |
| | no | | | |
| H5 | H4 | 2.45(11) | . | 2_655 |
| | no | | | |
| H6 | C13 | 2.88(7) | . | . |
| | no | | | |
| H6 | C14 | 3.07(7) | . | . |
| | no | | | |
| H8 | Pd | 3.60(6) | . | . |
| | no | | | |
| H8 | C13 | 3.00(6) | . | . |
| | no | | | |
| H9 | Cl | 3.08(6) | . | 3_565 |
| | no | | | |
| H10 | Cl | 3.14(6) | . | 5_555 |
| | no | | | |
| H10 | C17 | 2.99(6) | . | 6_555 |
| | no | | | |
| H11 | Cl | 2.99(7) | . | 5_555 |
| | no | | | |
| H12 | C1 | 2.64(6) | . | . |
| | no | | | |
| H12 | C2 | 2.99(6) | . | . |
| | no | | | |
| H12 | C24 | 2.82(6) | . | 5_555 |
| | no | | | |
| H12 | H24 | 2.54(8) | . | 5_555 |
| | no | | | |
| H14 | C7 | 2.90(7) | . | . |
| | no | | | |
| H14 | C21 | 2.98(8) | . | 6_555 |
| | no | | | |
| H15 | C3 | 2.95(6) | . | 6_555 |
| | no | | | |

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          no
 H17     C19         2.76(6)                     .       .
          no
 H17     H19         2.32(7)                     .       .
          no
 H17     Pd          3.31(6)                     .     2_555
          no
 H17     Cl          2.66(5)                     .     2_555
          no
 H19     C17         2.58(4)                     .       .
          no
 H19     H17         2.32(7)                     .       .
          no
 H19     C19         2.81(6)                     .     2_555
          no
 H19     C20         2.90(6)                     .     2_555
          no
 H19     C25         2.80(5)                     .     2_555
          no
 H19     C10         3.08(6)                     .     6_545
          no
 H19     C11         3.06(5)                     .     6_545
          no
 H21     Pd          2.72(6)                     .       .
          no
 H21     N           2.69(6)                     .       .
          no
 H22     Cl          2.87(6)                     .     3_555
          no
 H22     C22         2.81(5)                     .     3_555
          no
 H22     H22         2.48(8)                     .     3_555
          no
 H23     Pd          3.62(7)                     .     3_555
          no
 H23     C26         3.05(7)                     .     3_555
          no
 H24     C24         2.56(5)                     .     2_555
          no
 H24     H24         2.17(8)                     .     2_555
          no
 H24     H12         2.54(8)                     .     5_445
          no
 H26"    C3          2.90(9)                     .     7_555
          no
 H26"    H3         2.52(12)                     .     7_555
          no

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_geom_angle_DHA
_geom_contact_site_symmetry_A
#
#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
#
C17     H17     Cl          .86(6)    2.66(5)   3.402(6)
144(5)   2_555

# End of Crystallographic Information File
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#=== COMPLEX 6
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data_s1420c

#======================================================================

# 5. CHEMICAL DATA

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;
 ?
;
_chemical_name_common                 ?
_chemical_melting_point               ?
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_chemical_formula_structural          ?
# Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2O)'
_chemical_formula_sum                 '?'
_chemical_formula_weight                1203.38
_chemical_compound_source             ?

loop_
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_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
Pd  Pd   -0.9988    1.0072
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 P   P    0.1023    0.0942
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 N   N    0.0061    0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Cl  Cl    0.1484    0.1585
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 H   H    0.0000    0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 C   C    0.0033    0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#======================================================================

# 6. CRYSTAL DATA

_symmetry_cell_setting                  Triclinic
_symmetry_space_group_name_H-M       'P -1'

loop_
_symmetry_equiv_pos_as_xyz
 x,y,z
 -x,-y,-z

_cell_length_a                         15.1653(18)
_cell_length_b                           19.369(2)
_cell_length_c                         20.3003(17)
_cell_angle_alpha                       100.755(9)
_cell_angle_beta                         99.828(8)
_cell_angle_gamma                      111.470(10)
_cell_volume                            5262.1(11)
_cell_formula_units_Z                     2
_cell_measurement_temperature          150

_exptl_crystal_description          block
_exptl_crystal_colour               orange
_exptl_crystal_size_max              0.70
_exptl_crystal_size_mid              0.70
```

```
_exptl_crystal_size_min             0.45
_exptl_crystal_density_meas         'Not Measured'
_exptl_crystal_density_diffrn           1.519
_exptl_crystal_density_method        ?
_exptl_crystal_F_000                     2436
_exptl_absorpt_coefficient_mu            0.91
_exptl_absorpt_correction_type      none

#=============================================================

# 7. EXPERIMENTAL DATA

_exptl_special_details
; ?
;
_diffrn_ambient_temperature         150
_diffrn_radiation_wavelength           0.71073
_diffrn_radiation_type               'Mo K\a'
_diffrn_radiation_source             'Rotating Anode'
_diffrn_radiation_monochromator     Graphite

_diffrn_measurement_device_type      'CAD4T'
_diffrn_measurement_method           '\w-scan'


# number of measured reflections (redundant set)
_diffrn_reflns_number               ?
_diffrn_reflns_av_R_equivalents       0.0794
_diffrn_reflns_av_sigmaI/netI         0.1009
_diffrn_reflns_limit_h_min             -18
_diffrn_reflns_limit_h_max              16
_diffrn_reflns_limit_k_min               0
_diffrn_reflns_limit_k_max              23
_diffrn_reflns_limit_l_min             -24
_diffrn_reflns_limit_l_max              24
_diffrn_reflns_theta_min              1.06
_diffrn_reflns_theta_max             25.36

# number of unique reflections
_reflns_number_total                19488
# number of observed reflections (> n sig(I))
_reflns_number_gt                   11771
_reflns_threshold_expression         >2sigma(i)

_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_publication_material      'PLATON (Spek, 1990)'

#=============================================================

# 8. REFINEMENT DATA

_refine_ls_structure_factor_coef     Fsqd
_refine_ls_matrix_type               full
_refine_ls_weighting_scheme
'CALC W=1/[\S^2^(FO^2^)+(0.0675P)^2^+18.2225P] WHERE P=(FO^2^+2FC^2^)/3'
_refine_ls_hydrogen_treatment        'H-atom refinement: see text'
_refine_ls_number_reflns            18889
_refine_ls_number_parameters              1331
_refine_ls_number_restraints                 1
_refine_ls_R_factor_all                 0.1245
_refine_ls_R_factor_gt                  0.0673
_refine_ls_wR_factor_ref                0.1735
_refine_ls_wR_factor_gt                 0.1421
_refine_ls_goodness_of_fit_ref           1.008
_refine_ls_restrained_S_all              1.008
_refine_ls_shift/su_max                  0.007
_refine_ls_shift/su_mean                 0.000
```

```
_refine_diff_density_max                1.168
_refine_diff_density_min               -1.082
_refine_diff_density_rms                0.142

#=============================================================

# 9. ATOMIC COORDINATES AND THERMAL PARAMETERS

loop_
_atom_site_label
_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
 Pd1     Uani    0.15699(4)   0.23185(3)   0.68334(3)     1.000
0.0154(2)
 Cl1     Uani   0.11967(13)  0.17999(10)   0.79988(9)     1.000
0.0234(6)
 P1      Uani  -0.00609(13)  0.18941(10)   0.64312(9)     1.000
0.0159(5)
 P2      Uani   0.19177(13)  0.35886(10)   0.70101(9)     1.000
0.0166(6)
 N1      Uani     0.3071(4)    0.2615(3)    0.7181(3)     1.000
0.0168(17)
 N2      Uani     0.1337(4)    0.1147(3)    0.6358(3)     1.000
0.0158(17)
 C11     Uani     0.1072(5)    0.3885(4)    0.6511(4)     1.000
0.021(2)
 C21     Uani     0.0610(5)    0.4311(4)    0.6823(4)     1.000
0.026(2)
 C31     Uani    -0.0032(5)    0.4531(4)    0.6416(5)     1.000
0.030(3)
 C41     Uani    -0.0213(6)    0.4313(5)    0.5705(5)     1.000
0.040(3)
 C51     Uani     0.0221(6)    0.3881(5)    0.5389(5)     1.000
0.040(3)
 C61     Uani     0.0869(6)    0.3681(4)    0.5796(4)     1.000
0.028(3)
 C71     Uani     0.2201(5)    0.4127(4)    0.7914(3)     1.000
0.0158(19)
 C81     Uani     0.2048(6)    0.3738(4)    0.8421(4)     1.000
0.028(3)
 C91     Uani     0.2268(6)    0.4151(5)    0.9094(4)     1.000
0.037(3)
 C101    Uani     0.2647(6)    0.4947(5)    0.9285(4)     1.000
0.036(3)
 C111    Uani     0.2813(6)    0.5333(5)    0.8786(4)     1.000
0.029(3)
 C121    Uani     0.2593(5)    0.4926(4)    0.8095(4)     1.000
0.021(2)
 C131    Uani     0.3042(5)    0.4050(4)    0.6763(3)     1.000
0.017(2)
 C141    Uani     0.3189(5)    0.4709(4)    0.6517(4)     1.000
0.023(2)
 C151    Uani     0.4061(5)    0.5115(4)    0.6373(4)     1.000
0.026(3)
 C161    Uani     0.4815(5)    0.4868(4)    0.6462(4)     1.000
0.023(2)
 C171    Uani     0.4695(5)    0.4224(4)    0.6704(4)     1.000
0.023(2)
 C181    Uani     0.3816(5)    0.3810(4)    0.6853(4)     1.000
0.021(2)
 C191    Uani     0.3814(5)    0.3175(4)    0.7131(4)     1.000
0.019(2)
 C201    Uani     0.3339(5)    0.2093(4)    0.7523(4)     1.000
```

0.019(2)
 C211    Uani     0.3690(5)    0.2320(5)    0.8239(4)     1.000
0.027(3)
 C221    Uani     0.4042(6)    0.1858(5)    0.8556(4)     1.000
0.039(3)
 C231    Uani     0.4043(6)    0.1198(5)    0.8171(4)     1.000
0.035(3)
 C241    Uani     0.3686(5)    0.0982(4)    0.7464(4)     1.000
0.025(2)
 C251    Uani     0.3323(5)    0.1421(4)    0.7122(4)     1.000
0.018(2)
 C261    Uani     0.2998(5)    0.1188(4)    0.6359(4)     1.000
0.0183(19)
 C271    Uani     0.3603(6)    0.1040(4)    0.5968(4)     1.000
0.027(3)
 C281    Uani     0.3302(5)    0.0755(4)    0.5257(4)     1.000
0.026(3)
 C291    Uani     0.2361(5)    0.0626(4)    0.4908(4)     1.000
0.025(2)
 C301    Uani     0.1735(5)    0.0773(4)    0.5282(4)     1.000
0.022(2)
 C311    Uani     0.2045(5)    0.1047(4)    0.5993(4)     1.000
0.0173(19)
 C321    Uani     0.0621(5)    0.0514(4)    0.6330(3)     1.000
0.016(2)
 C331    Uani    -0.0260(5)    0.0428(4)    0.6565(4)     1.000
0.019(2)
 C341    Uani    -0.0733(5)   -0.0269(4)    0.6708(3)     1.000
0.018(2)
 C351    Uani    -0.1584(5)   -0.0419(4)    0.6934(4)     1.000
0.022(2)
 C361    Uani    -0.1962(6)    0.0135(4)    0.7012(4)     1.000
0.026(2)
 C371    Uani    -0.1496(5)    0.0824(4)    0.6857(4)     1.000
0.021(2)
 C381    Uani    -0.0638(5)    0.0991(4)    0.6638(3)     1.000
0.015(2)
 C391    Uani    -0.0639(5)    0.2475(4)    0.6809(4)     1.000
0.020(2)
 C401    Uani    -0.0434(5)    0.2686(4)    0.7527(4)     1.000
0.024(3)
 C411    Uani    -0.0915(6)    0.3083(4)    0.7852(5)     1.000
0.033(3)
 C421    Uani    -0.1579(6)    0.3274(5)    0.7462(5)     1.000
0.036(3)
 C431    Uani    -0.1782(5)    0.3068(4)    0.6747(4)     1.000
0.029(3)
 C441    Uani    -0.1317(5)    0.2671(4)    0.6411(4)     1.000
0.025(3)
 C451    Uani    -0.0461(5)    0.1657(4)    0.5494(4)     1.000
0.021(2)
 C461    Uani    -0.1451(6)    0.1284(4)    0.5143(4)     1.000
0.030(3)
 C471    Uani    -0.1746(7)    0.1128(5)    0.4434(4)     1.000
0.035(3)
 C481    Uani    -0.1049(7)    0.1331(5)    0.4068(4)     1.000
0.037(3)
 C491    Uani    -0.0064(7)    0.1683(5)    0.4401(4)     1.000
0.032(3)
 C501    Uani     0.0225(6)    0.1835(4)    0.5107(4)     1.000
0.029(3)
 Pd2     Uani    0.17064(4)   0.25634(3)   0.18083(3)     1.000
0.0157(2)
 P3      Uani   0.00681(13)  0.21212(10)   0.14163(9)     1.000
0.0169(6)
 P4      Uani   0.20516(13)  0.38369(10)  0.19723(10)     1.000
0.0173(6)

| | | | | | |
|---|---|---|---|---|---|
| N3 | Uani | 0.3221(4) | 0.2872(3) | 0.2146(3) | 1.000 |
| 0.0159(17) | | | | | |
| N4 | Uani | 0.1452(4) | 0.1375(3) | 0.1381(3) | 1.000 |
| 0.0184(17) | | | | | |
| C12 | Uani | 0.1179(5) | 0.4108(4) | 0.1473(4) | 1.000 |
| 0.020(2) | | | | | |
| C22 | Uani | 0.0764(5) | 0.4567(4) | 0.1796(4) | 1.000 |
| 0.025(3) | | | | | |
| C32 | Uani | 0.0092(6) | 0.4757(4) | 0.1396(4) | 1.000 |
| 0.030(3) | | | | | |
| C42 | Uani | -0.0148(6) | 0.4508(5) | 0.0682(5) | 1.000 |
| 0.035(3) | | | | | |
| C52 | Uani | 0.0274(6) | 0.4072(5) | 0.0363(4) | 1.000 |
| 0.033(3) | | | | | |
| C62 | Uani | 0.0938(6) | 0.3870(4) | 0.0752(4) | 1.000 |
| 0.028(3) | | | | | |
| C72 | Uani | 0.2343(5) | 0.4403(4) | 0.2870(4) | 1.000 |
| 0.018(2) | | | | | |
| C82 | Uani | 0.2100(6) | 0.4063(4) | 0.3388(4) | 1.000 |
| 0.027(3) | | | | | |
| C92 | Uani | 0.2297(7) | 0.4512(5) | 0.4052(4) | 1.000 |
| 0.042(3) | | | | | |
| C102 | Uani | 0.2768(6) | 0.5303(5) | 0.4213(4) | 1.000 |
| 0.034(3) | | | | | |
| C112 | Uani | 0.3034(6) | 0.5650(5) | 0.3691(4) | 1.000 |
| 0.030(3) | | | | | |
| C122 | Uani | 0.2818(5) | 0.5209(4) | 0.3027(4) | 1.000 |
| 0.023(3) | | | | | |
| C132 | Uani | 0.3174(5) | 0.4293(4) | 0.1713(4) | 1.000 |
| 0.019(2) | | | | | |
| C142 | Uani | 0.3283(6) | 0.4926(4) | 0.1445(4) | 1.000 |
| 0.030(3) | | | | | |
| C152 | Uani | 0.4163(6) | 0.5328(5) | 0.1293(4) | 1.000 |
| 0.031(3) | | | | | |
| C162 | Uani | 0.4930(6) | 0.5111(5) | 0.1412(4) | 1.000 |
| 0.029(3) | | | | | |
| C172 | Uani | 0.4827(5) | 0.4495(4) | 0.1689(4) | 1.000 |
| 0.021(2) | | | | | |
| C182 | Uani | 0.3952(5) | 0.4078(4) | 0.1832(4) | 1.000 |
| 0.019(2) | | | | | |
| C192 | Uani | 0.3939(5) | 0.3435(4) | 0.2116(4) | 1.000 |
| 0.019(2) | | | | | |
| C202 | Uani | 0.3497(5) | 0.2369(4) | 0.2509(3) | 1.000 |
| 0.017(2) | | | | | |
| C212 | Uani | 0.3863(6) | 0.2615(4) | 0.3218(4) | 1.000 |
| 0.027(3) | | | | | |
| C222 | Uani | 0.4221(6) | 0.2193(5) | 0.3577(4) | 1.000 |
| 0.030(3) | | | | | |
| C232 | Uani | 0.4196(5) | 0.1502(5) | 0.3200(4) | 1.000 |
| 0.032(3) | | | | | |
| C242 | Uani | 0.3826(5) | 0.1252(4) | 0.2489(4) | 1.000 |
| 0.025(3) | | | | | |
| C252 | Uani | 0.3446(5) | 0.1670(4) | 0.2126(4) | 1.000 |
| 0.018(2) | | | | | |
| C262 | Uani | 0.3089(5) | 0.1403(4) | 0.1362(4) | 1.000 |
| 0.021(2) | | | | | |
| C272 | Uani | 0.3692(6) | 0.1234(5) | 0.0969(4) | 1.000 |
| 0.031(3) | | | | | |
| C282 | Uani | 0.3379(6) | 0.0938(5) | 0.0261(4) | 1.000 |
| 0.037(3) | | | | | |
| C292 | Uani | 0.2431(6) | 0.0785(5) | -0.0075(4) | 1.000 |
| 0.031(3) | | | | | |
| C302 | Uani | 0.1808(6) | 0.0944(4) | 0.0290(4) | 1.000 |
| 0.026(3) | | | | | |
| C312 | Uani | 0.2148(5) | 0.1256(4) | 0.1000(4) | 1.000 |
| 0.021(2) | | | | | |
| C322 | Uani | 0.0753(5) | 0.0764(4) | 0.1375(4) | 1.000 |

0.019(2)
 C332  Uani  -0.0123(5)  0.0686(4)  0.1623(4)  1.000
0.019(2)
 C342  Uani  -0.0606(5)  0.0002(4)  0.1769(4)  1.000
0.021(2)
 C352  Uani  -0.1445(5)  -0.0118(4)  0.2008(4)  1.000
0.023(2)
 C362  Uani  -0.1793(6)  0.0436(4)  0.2093(4)  1.000
0.027(3)
 C372  Uani  -0.1325(5)  0.1126(4)  0.1933(4)  1.000
0.022(2)
 C382  Uani  -0.0489(5)  0.1266(4)  0.1703(3)  1.000
0.016(2)
 C392  Uani  -0.0555(5)  0.2700(4)  0.1711(4)  1.000
0.017(2)
 C402  Uani  -0.0370(5)  0.3000(4)  0.2418(4)  1.000
0.025(3)
 C412  Uani  -0.0850(6)  0.3418(4)  0.2680(5)  1.000
0.031(3)
 C422  Uani  -0.1543(6)  0.3532(5)  0.2230(5)  1.000
0.036(3)
 C432  Uani  -0.1733(6)  0.3250(4)  0.1536(5)  1.000
0.036(3)
 C442  Uani  -0.1244(5)  0.2832(4)  0.1252(4)  1.000
0.024(2)
 C452  Uani  -0.0368(5)  0.1760(4)  0.0474(4)  1.000
0.024(2)
 C462  Uani  -0.1345(6)  0.1277(4)  0.0154(4)  1.000
0.028(3)
 C472  Uani  -0.1650(7)  0.1007(5)  -0.0560(5)  1.000
0.042(3)
 C482  Uani  -0.0974(8)  0.1217(5)  -0.0951(5)  1.000
0.043(3)
 C492  Uani  -0.0022(7)  0.1685(5)  -0.0645(4)  1.000
0.037(3)
 C502  Uani  0.0297(6)  0.1962(4)  0.0071(4)  1.000
0.027(3)
 Cl19  Uani  0.2174(2)  0.61731(16)  0.08744(14)  1.000
0.0618(10)
 Cl20  Uiso  0.3363(7)  0.7527(10)  0.0411(7)  0.52(3)
0.078(4)
 C7  Uani  0.3216(10)  0.7045(6)  0.1053(6)  1.000
0.080(5)
 Cl22  Uiso  0.3472(17)  0.710(2)  0.0286(8)  0.32(3)
0.114(11)
 Cl21  Uiso  0.265(3)  0.7661(12)  0.0837(13)  0.158(10)
0.118(15)
 Cl15  Uiso  0.5375(5)  0.0239(3)  0.6745(4)  0.607(14)
0.073(2)
 Cl16  Uiso  0.6847(7)  0.1209(5)  0.7991(3)  0.607(14)
0.080(3)
 C6  Uani  0.6198(8)  0.1207(6)  0.7255(6)  1.000
0.064(4)
 Cl18  Uiso  0.5951(11)  0.0685(10)  0.6510(5)  0.393(14)
0.097(6)
 Cl17  Uiso  0.6228(17)  0.0824(13)  0.7981(9)  0.393(14)
0.139(7)
 Cl5  Uani  0.3221(3)  0.25552(16)  0.51623(16)  1.000
0.0908(16)
 Cl6  Uani  0.4414(2)  0.39167(15)  0.48132(13)  1.000
0.0719(10)
 C1  Uani  0.3236(8)  0.3298(5)  0.4810(5)  1.000
0.058(4)
 Cl7  Uani  0.4825(2)  0.37123(19)  -0.00543(14)  1.000
0.0870(11)
 Cl8  Uani  0.2955(2)  0.28631(18)  0.01782(16)  1.000
0.0765(11)

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | Uani | 0.4161(8) | 0.2974(6) | 0.0286(5) | 1.000 | 0.059(4) |
| Cl9 | Uani | 0.7668(2) | 0.38243(18) | 0.39270(15) | 1.000 | 0.0667(11) |
| Cl10 | Uani | 0.7490(3) | 0.2262(2) | 0.3477(2) | 1.000 | 0.108(2) |
| C3 | Uani | 0.6908(8) | 0.2884(7) | 0.3396(6) | 1.000 | 0.068(5) |
| Cl11 | Uani | 0.6581(2) | 0.26230(14) | 0.50181(12) | 1.000 | 0.0542(9) |
| Cl12 | Uani | 0.5820(3) | 0.10729(19) | 0.5127(3) | 1.000 | 0.144(3) |
| C4 | Uani | 0.5816(8) | 0.1974(5) | 0.5376(5) | 1.000 | 0.057(4) |
| Cl13 | Uani | 0.6147(4) | 0.1047(3) | 0.0567(4) | 1.000 | 0.181(4) |
| Cl14 | Uani | 0.5783(3) | 0.0731(3) | 0.1846(4) | 1.000 | 0.161(3) |
| C5 | Uani | 0.6322(9) | 0.1416(9) | 0.1446(13) | 1.000 | 0.155(11) |
| Cl2 | Uani | 0.13642(13) | 0.21416(10) | 0.30874(9) | 1.000 | 0.0246(6) |
| Cl3 | Uani | 0.41078(14) | 0.71306(11) | 0.28358(11) | 1.000 | 0.0338(7) |
| Cl4 | Uani | 0.58694(15) | 0.30788(13) | 0.18176(13) | 1.000 | 0.0445(8) |
| H21 | Uiso | 0.0731(11) | 0.4453(12) | 0.732(4) | 1.000 | 0.0310 |
| H31 | Uiso | -0.035(3) | 0.484(3) | 0.6636(19) | 1.000 | 0.0360 |
| H41 | Uiso | -0.061(4) | 0.4453(15) | 0.545(3) | 1.000 | 0.0480 |
| H51 | Uiso | 0.0099(14) | 0.3746(16) | 0.497(5) | 1.000 | 0.0470 |
| H61 | Uiso | 0.120(3) | 0.338(2) | 0.5564(18) | 1.000 | 0.0330 |
| H81 | Uiso | 0.178(2) | 0.317(5) | 0.8297(11) | 1.000 | 0.0330 |
| H91 | Uiso | 0.2168(12) | 0.391(3) | 0.941(3) | 1.000 | 0.0450 |
| H101 | Uiso | 0.27870 | 0.52180 | 0.97460 | 1.000 | 0.0420 |
| H111 | Uiso | 0.308(2) | 0.588(5) | 0.8912(11) | 1.000 | 0.0340 |
| H121 | Uiso | 0.2690(10) | 0.515(2) | 0.781(3) | 1.000 | 0.0260 |
| H141 | Uiso | 0.269(4) | 0.4872(14) | 0.6451(7) | 1.000 | 0.0280 |
| H151 | Uiso | 0.4150(9) | 0.559(4) | 0.6206(13) | 1.000 | 0.0310 |
| H161 | Uiso | 0.542(5) | 0.515(2) | 0.6356(9) | 1.000 | 0.0280 |
| H171 | Uiso | 0.515(4) | 0.4083(14) | 0.6761(6) | 1.000 | 0.0280 |
| H191 | Uiso | 0.438(5) | 0.3173(4) | 0.7282(13) | 1.000 | 0.0230 |
| H211 | Uiso | 0.3691(5) | 0.277(4) | 0.850(2) | 1.000 | 0.0320 |
| H221 | Uiso | 0.424(2) | 0.1976(15) | 0.895(5) | 1.000 | 0.0470 |
| H231 | Uiso | 0.426(2) | 0.093(3) | 0.837(2) | 1.000 | 0.0420 |
| H241 | Uiso | 0.3686(5) | 0.050(4) | 0.719(2) | 1.000 | 0.0300 |
| H271 | Uiso | 0.417(6) | 0.1125(9) | 0.617(2) | 1.000 | 0.0330 |
| H281 | Uiso | 0.373(4) | 0.0650(10) | 0.501(2) | 1.000 | |

| | | | | | |
|---|---|---|---|---|---|
| | | | | | 0.0310 |
| H291 | Uiso | 0.2165(18) | 0.0454(16) | 0.446(4) | 1.000 |
| | | | | | 0.0300 |
| H301 | Uiso | 0.107(5) | 0.0681(8) | 0.5039(19) | 1.000 |
| | | | | | 0.0270 |
| H321 | Uiso | 0.0671(6) | 0.006(4) | 0.6139(15) | 1.000 |
| | | | | | 0.0200 |
| H341 | Uiso | -0.047(2) | -0.065(3) | 0.6650(6) | 1.000 |
| | | | | | 0.0220 |
| H351 | Uiso | -0.190(3) | -0.089(4) | 0.7033(9) | 1.000 |
| | | | | | 0.0270 |
| H361 | Uiso | -0.253(5) | 0.0045(9) | 0.7166(14) | 1.000 |
| | | | | | 0.0310 |
| H371 | Uiso | -0.175(2) | 0.116(3) | 0.6898(5) | 1.000 |
| | | | | | 0.0250 |
| H401 | Uiso | 0.005(4) | 0.2558(11) | 0.781(2) | 1.000 |
| | | | | | 0.0290 |
| H411 | Uiso | -0.0787(13) | 0.3218(13) | 0.833(4) | 1.000 |
| | | | | | 0.0400 |
| H421 | Uiso | -0.188(3) | 0.354(3) | 0.767(2) | 1.000 |
| | | | | | 0.0430 |
| H431 | Uiso | -0.224(4) | 0.3198(12) | 0.649(2) | 1.000 |
| | | | | | 0.0350 |
| H441 | Uiso | -0.1455(12) | 0.2533(12) | 0.591(4) | 1.000 |
| | | | | | 0.0300 |
| H461 | Uiso | -0.193(4) | 0.1136(13) | 0.540(2) | 1.000 |
| | | | | | 0.0350 |
| H471 | Uiso | -0.245(6) | 0.087(2) | 0.419(2) | 1.000 |
| | | | | | 0.0420 |
| H481 | Uiso | -0.122(2) | 0.1245(11) | 0.366(5) | 1.000 |
| | | | | | 0.0450 |
| H491 | Uiso | 0.032(4) | 0.1790(13) | 0.420(2) | 1.000 |
| | | | | | 0.0390 |
| H501 | Uiso | 0.086(6) | 0.205(2) | 0.532(2) | 1.000 |
| | | | | | 0.0350 |
| H22 | Uiso | 0.0934(15) | 0.4744(15) | 0.228(4) | 1.000 |
| | | | | | 0.0290 |
| H32 | Uiso | -0.020(3) | 0.506(3) | 0.1614(19) | 1.000 |
| | | | | | 0.0360 |
| H42 | Uiso | -0.062(4) | 0.4643(12) | 0.040(2) | 1.000 |
| | | | | | 0.0420 |
| H52 | Uiso | 0.0129(16) | 0.3926(15) | -0.007(4) | 1.000 |
| | | | | | 0.0400 |
| H62 | Uiso | 0.123(3) | 0.357(3) | 0.0528(19) | 1.000 |
| | | | | | 0.0340 |
| H82 | Uiso | 0.179(3) | 0.351(5) | 0.3287(9) | 1.000 |
| | | | | | 0.0330 |
| H92 | Uiso | 0.214(2) | 0.432(2) | 0.434(3) | 1.000 |
| | | | | | 0.0500 |
| H102 | Uiso | 0.2914(14) | 0.562(3) | 0.469(4) | 1.000 |
| | | | | | 0.0410 |
| H112 | Uiso | 0.337(3) | 0.621(5) | 0.3799(10) | 1.000 |
| | | | | | 0.0360 |
| H122 | Uiso | 0.2973(15) | 0.543(2) | 0.270(3) | 1.000 |
| | | | | | 0.0270 |
| H142 | Uiso | 0.280(5) | 0.5070(14) | 0.1372(8) | 1.000 |
| | | | | | 0.0360 |
| H152 | Uiso | 0.4229(8) | 0.574(4) | 0.1112(17) | 1.000 |
| | | | | | 0.0370 |
| H162 | Uiso | 0.550(5) | 0.537(2) | 0.1310(10) | 1.000 |
| | | | | | 0.0350 |
| H172 | Uiso | 0.538(4) | 0.4349(12) | 0.1786(8) | 1.000 |
| | | | | | 0.0250 |
| H192 | Uiso | 0.456(5) | 0.3447(4) | 0.2302(15) | 1.000 |
| | | | | | 0.0230 |
| H212 | Uiso | 0.3871(6) | 0.307(4) | 0.346(2) | 1.000 |
| | | | | | 0.0320 |

| | | | | | | |
|---|---|---|---|---|---|---|
| H222 | Uiso | 0.449(2) | 0.2373(16) | 0.408(4) | 1.000 | 0.0360 |
| H232 | Uiso | 0.440(2) | 0.125(3) | 0.340(2) | 1.000 | 0.0390 |
| H242 | Uiso | 0.3829(5) | 0.077(4) | 0.223(2) | 1.000 | 0.0300 |
| H272 | Uiso | 0.425(6) | 0.1314(9) | 0.117(2) | 1.000 | 0.0370 |
| H282 | Uiso | 0.382(4) | 0.0837(10) | 0.000(2) | 1.000 | 0.0440 |
| H292 | Uiso | 0.223(2) | 0.0590(19) | -0.051(4) | 1.000 | 0.0380 |
| H302 | Uiso | 0.120(5) | 0.0848(10) | 0.007(2) | 1.000 | 0.0320 |
| H322 | Uiso | 0.0800(6) | 0.031(4) | 0.1191(15) | 1.000 | 0.0230 |
| H342 | Uiso | -0.0404(19) | -0.033(3) | 0.1717(6) | 1.000 | 0.0250 |
| H352 | Uiso | -0.175(3) | -0.055(4) | 0.2103(9) | 1.000 | 0.0280 |
| H362 | Uiso | -0.235(5) | 0.0355(8) | 0.2259(15) | 1.000 | 0.0320 |
| H372 | Uiso | -0.159(2) | 0.152(3) | 0.1985(5) | 1.000 | 0.0270 |
| H402 | Uiso | 0.002(4) | 0.2929(8) | 0.268(3) | 1.000 | 0.0300 |
| H412 | Uiso | -0.0710(14) | 0.3626(19) | 0.316(4) | 1.000 | 0.0370 |
| H422 | Uiso | -0.189(3) | 0.381(3) | 0.2408(17) | 1.000 | 0.0430 |
| H432 | Uiso | -0.216(4) | 0.3329(9) | 0.127(3) | 1.000 | 0.0430 |
| H442 | Uiso | -0.1379(12) | 0.2633(16) | 0.074(4) | 1.000 | 0.0290 |
| H462 | Uiso | -0.179(4) | 0.1137(13) | 0.042(2) | 1.000 | 0.0340 |
| H472 | Uiso | -0.231(6) | 0.069(3) | -0.078(2) | 1.000 | 0.0500 |
| H482 | Uiso | -0.120(2) | 0.1019(19) | -0.147(5) | 1.000 | 0.0520 |
| H492 | Uiso | 0.039(4) | 0.1811(14) | -0.090(3) | 1.000 | 0.0430 |
| H502 | Uiso | 0.093(6) | 0.227(3) | 0.0278(18) | 1.000 | 0.0320 |
| H320 | Uiso | 0.37920 | 0.69410 | 0.11760 | 0.52(3) | 0.1080 |
| H310 | Uiso | 0.32120 | 0.73960 | 0.14610 | 0.52(3) | 0.1080 |
| H330 | Uiso | 0.36490 | 0.70000 | 0.07620 | 0.158(10) | 0.1080 |
| H340 | Uiso | 0.35790 | 0.72210 | 0.15380 | 0.158(10) | 0.1080 |
| H350 | Uiso | 0.30790 | 0.74790 | 0.12500 | 0.32(3) | 0.1080 |
| H360 | Uiso | 0.37640 | 0.70450 | 0.13780 | 0.32(3) | 0.1080 |
| H620 | Uiso | 0.58190 | 0.15050 | 0.73510 | 0.607(14) | 0.0870 |
| H610 | Uiso | 0.66370 | 0.14500 | 0.69900 | 0.607(14) | 0.0870 |
| H630 | Uiso | 0.57260 | 0.14360 | 0.72540 | 0.393(14) | 0.0870 |
| H640 | Uiso | 0.68360 | 0.16250 | 0.73370 | 0.393(14) | 0.0870 |
| H11 | Uiso | 0.29500 | 0.35940 | 0.50700 | 1.000 | 0.0780 |
| H201 | Uiso | 0.28300 | 0.30850 | 0.43350 | 1.000 | |

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  0.0780
 H12     Uiso       0.44710      0.30950      0.07770     1.000
  0.0790
 H202    Uiso       0.41740      0.24940      0.00550     1.000
  0.0790
 H13     Uiso       0.62960      0.26950      0.35280     1.000
  0.0910
 H203    Uiso       0.67570      0.28960      0.29150     1.000
  0.0910
 H14     Uiso       0.60310      0.21640      0.58790     1.000
  0.0770
 H204    Uiso       0.51520      0.19350      0.52290     1.000
  0.0770
 H15     Uiso       0.70210      0.16690      0.16680     1.000
  0.2090
 H205    Uiso       0.60570      0.18030      0.15100     1.000
  0.2090

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
  Pd1      0.0145(3)  0.0131(3)  0.0217(3)   0.0063(2)
0.0057(2)   0.0079(2)
  Cl1     0.0297(10)  0.0212(9) 0.0259(10)   0.0121(8)
0.0112(8)   0.0131(8)
  P1       0.0153(9)  0.0153(9) 0.0222(10)   0.0081(8)
0.0069(8)   0.0094(8)
  P2       0.0177(9) 0.0164(10) 0.0209(10)   0.0072(8)
0.0077(8)   0.0105(8)
  N1        0.014(3)   0.014(3)   0.021(3)    0.001(2)
0.002(2)    0.007(3)
  N2        0.017(3)   0.021(3)   0.013(3)    0.009(2)
0.001(2)    0.011(3)
  C11       0.020(4)   0.020(4)   0.028(4)    0.010(3)
0.008(3)    0.010(3)
  C21       0.025(4)   0.024(4)   0.028(4)    0.006(3)
0.003(3)    0.012(3)
  C31       0.022(4)   0.021(4)   0.055(6)    0.014(4)
0.009(4)    0.015(3)
  C41       0.035(5)   0.037(5)   0.056(6)    0.028(5)
-0.001(4)    0.023(4)
  C51       0.039(5)   0.037(5)   0.040(5)    0.016(4)
-0.002(4)    0.015(4)
  C61       0.033(5)   0.032(5)   0.030(5)    0.018(4)
0.011(4)    0.021(4)
  C71       0.009(3)   0.011(3)   0.021(4)    0.001(3)
0.001(3)    0.000(3)
  C81       0.040(5)   0.016(4)   0.028(4)    0.009(3)
0.012(4)    0.010(4)
  C91       0.054(6)   0.030(5)   0.029(5)    0.018(4)
0.016(4)    0.011(4)
  C101      0.043(5)   0.034(5)   0.026(5)   -0.001(4)
0.009(4)    0.016(4)
  C111      0.026(4)   0.028(4)   0.028(5)    0.000(4)
0.004(3)    0.012(4)
  C121      0.016(4)   0.022(4)   0.034(4)    0.011(3)
0.009(3)    0.014(3)
  C131      0.016(4)   0.010(3)   0.020(4)    0.002(3)
0.005(3)    0.002(3)
  C141      0.027(4)   0.016(4)   0.032(4)    0.006(3)
0.008(3)    0.014(3)
  C151      0.027(4)   0.022(4)   0.035(5)    0.021(4)
```

| | | | | |
|---|---|---|---|---|
| 0.012(4) | 0.010(3) | | | |
| C161 | 0.020(4) | 0.020(4) | 0.021(4) | 0.006(3) |
| 0.007(3) | -0.002(3) | | | |
| C171 | 0.021(4) | 0.028(4) | 0.022(4) | 0.010(3) |
| 0.009(3) | 0.009(3) | | | |
| C181 | 0.019(4) | 0.013(4) | 0.029(4) | 0.005(3) |
| 0.004(3) | 0.007(3) | | | |
| C191 | 0.014(4) | 0.023(4) | 0.022(4) | 0.004(3) |
| 0.004(3) | 0.011(3) | | | |
| C201 | 0.021(4) | 0.012(4) | 0.027(4) | 0.009(3) |
| 0.012(3) | 0.005(3) | | | |
| C211 | 0.025(4) | 0.032(5) | 0.026(4) | 0.010(4) |
| 0.002(3) | 0.016(4) | | | |
| C221 | 0.041(5) | 0.053(6) | 0.024(5) | 0.015(4) |
| 0.000(4) | 0.022(5) | | | |
| C231 | 0.038(5) | 0.035(5) | 0.046(6) | 0.023(4) |
| 0.012(4) | 0.023(4) | | | |
| C241 | 0.025(4) | 0.027(4) | 0.031(4) | 0.013(3) |
| 0.011(3) | 0.017(3) | | | |
| C251 | 0.013(4) | 0.020(4) | 0.021(4) | 0.008(3) |
| 0.002(3) | 0.007(3) | | | |
| C261 | 0.012(3) | 0.011(3) | 0.027(4) | 0.008(3) |
| 0.005(3) | -0.002(3) | | | |
| C271 | 0.020(4) | 0.024(4) | 0.040(5) | 0.010(4) |
| 0.010(4) | 0.011(3) | | | |
| C281 | 0.021(4) | 0.028(4) | 0.031(5) | 0.004(3) |
| 0.013(4) | 0.012(3) | | | |
| C291 | 0.024(4) | 0.019(4) | 0.026(4) | -0.001(3) |
| 0.005(3) | 0.006(3) | | | |
| C301 | 0.022(4) | 0.015(4) | 0.024(4) | 0.000(3) |
| 0.001(3) | 0.007(3) | | | |
| C311 | 0.011(3) | 0.012(3) | 0.031(4) | 0.005(3) |
| 0.009(3) | 0.006(3) | | | |
| C321 | 0.017(4) | 0.017(4) | 0.022(4) | 0.007(3) |
| 0.006(3) | 0.013(3) | | | |
| C331 | 0.019(4) | 0.021(4) | 0.020(4) | 0.009(3) |
| 0.004(3) | 0.010(3) | | | |
| C341 | 0.022(4) | 0.012(4) | 0.022(4) | 0.006(3) |
| 0.006(3) | 0.007(3) | | | |
| C351 | 0.019(4) | 0.016(4) | 0.030(4) | 0.011(3) |
| 0.005(3) | 0.003(3) | | | |
| C361 | 0.028(4) | 0.025(4) | 0.028(4) | 0.009(3) |
| 0.011(4) | 0.011(4) | | | |
| C371 | 0.020(4) | 0.014(4) | 0.033(4) | 0.009(3) |
| 0.011(3) | 0.008(3) | | | |
| C381 | 0.018(4) | 0.008(3) | 0.022(4) | 0.001(3) |
| 0.008(3) | 0.008(3) | | | |
| C391 | 0.015(4) | 0.017(4) | 0.033(4) | 0.011(3) |
| 0.009(3) | 0.010(3) | | | |
| C401 | 0.022(4) | 0.017(4) | 0.036(5) | 0.007(3) |
| 0.012(3) | 0.010(3) | | | |
| C411 | 0.035(5) | 0.029(5) | 0.034(5) | 0.000(4) |
| 0.014(4) | 0.013(4) | | | |
| C421 | 0.024(4) | 0.032(5) | 0.052(6) | -0.002(4) |
| 0.008(4) | 0.018(4) | | | |
| C431 | 0.013(4) | 0.024(4) | 0.049(5) | 0.003(4) |
| 0.002(4) | 0.013(3) | | | |
| C441 | 0.017(4) | 0.023(4) | 0.035(5) | 0.008(3) |
| 0.004(3) | 0.008(3) | | | |
| C451 | 0.022(4) | 0.019(4) | 0.026(4) | 0.010(3) |
| 0.008(3) | 0.011(3) | | | |
| C461 | 0.026(4) | 0.019(4) | 0.041(5) | 0.007(4) |
| 0.004(4) | 0.009(3) | | | |
| C471 | 0.044(5) | 0.031(5) | 0.027(5) | 0.006(4) |
| 0.000(4) | 0.018(4) | | | |
| C481 | 0.065(7) | 0.028(5) | 0.022(4) | 0.006(4) |
| 0.003(4) | 0.026(5) | | | |

| | | | | | |
|---|---|---|---|---|---|
| C491 | 0.054(6) | 0.039(5) | 0.023(4) | 0.020(4) | 0.025(4) | 0.030(5) |
| C501 | 0.035(5) | 0.019(4) | 0.035(5) | 0.006(3) | 0.012(4) | 0.012(4) |
| Pd2 | 0.0144(3) | 0.0149(3) | 0.0219(3) | 0.0080(2) | 0.0053(2) | 0.0087(2) |
| P3 | 0.0156(9) | 0.0191(10) | 0.0219(10) | 0.0086(8) | 0.0074(8) | 0.0111(8) |
| P4 | 0.0166(9) | 0.0164(10) | 0.0253(10) | 0.0109(8) | 0.0085(8) | 0.0100(8) |
| N3 | 0.016(3) | 0.010(3) | 0.017(3) | 0.003(2) | -0.001(2) | 0.003(3) |
| N4 | 0.014(3) | 0.018(3) | 0.024(3) | 0.004(3) | 0.003(3) | 0.009(3) |
| C12 | 0.019(4) | 0.014(4) | 0.029(4) | 0.011(3) | 0.006(3) | 0.007(3) |
| C22 | 0.022(4) | 0.024(4) | 0.034(5) | 0.014(3) | 0.013(3) | 0.011(3) |
| C32 | 0.027(4) | 0.027(4) | 0.042(5) | 0.010(4) | 0.002(4) | 0.019(4) |
| C42 | 0.036(5) | 0.035(5) | 0.046(6) | 0.021(4) | 0.007(4) | 0.025(4) |
| C52 | 0.042(5) | 0.035(5) | 0.027(5) | 0.018(4) | 0.008(4) | 0.016(4) |
| C62 | 0.033(5) | 0.021(4) | 0.032(5) | 0.011(3) | 0.008(4) | 0.012(4) |
| C72 | 0.014(4) | 0.015(4) | 0.026(4) | 0.004(3) | 0.002(3) | 0.008(3) |
| C82 | 0.037(5) | 0.015(4) | 0.031(5) | 0.011(3) | 0.006(4) | 0.011(3) |
| C92 | 0.069(7) | 0.036(5) | 0.027(5) | 0.013(4) | 0.023(5) | 0.022(5) |
| C102 | 0.039(5) | 0.028(5) | 0.027(5) | 0.001(4) | -0.002(4) | 0.013(4) |
| C112 | 0.023(4) | 0.023(4) | 0.040(5) | -0.001(4) | 0.001(4) | 0.013(3) |
| C122 | 0.016(4) | 0.023(4) | 0.034(5) | 0.012(4) | 0.008(3) | 0.011(3) |
| C132 | 0.015(4) | 0.019(4) | 0.028(4) | 0.009(3) | 0.010(3) | 0.009(3) |
| C142 | 0.029(4) | 0.031(5) | 0.045(5) | 0.022(4) | 0.018(4) | 0.019(4) |
| C152 | 0.029(5) | 0.030(5) | 0.043(5) | 0.026(4) | 0.018(4) | 0.012(4) |
| C162 | 0.026(4) | 0.033(5) | 0.037(5) | 0.018(4) | 0.019(4) | 0.014(4) |
| C172 | 0.021(4) | 0.019(4) | 0.021(4) | 0.005(3) | 0.003(3) | 0.006(3) |
| C182 | 0.021(4) | 0.019(4) | 0.019(4) | 0.005(3) | 0.004(3) | 0.010(3) |
| C192 | 0.019(4) | 0.019(4) | 0.024(4) | 0.008(3) | 0.006(3) | 0.012(3) |
| C202 | 0.013(3) | 0.022(4) | 0.016(4) | 0.010(3) | 0.003(3) | 0.005(3) |
| C212 | 0.033(5) | 0.023(4) | 0.030(4) | 0.012(3) | 0.009(4) | 0.015(4) |
| C222 | 0.030(5) | 0.040(5) | 0.027(4) | 0.020(4) | 0.005(4) | 0.018(4) |
| C232 | 0.024(4) | 0.043(5) | 0.049(6) | 0.036(5) | 0.012(4) | 0.023(4) |
| C242 | 0.015(4) | 0.025(4) | 0.039(5) | 0.010(4) | 0.005(3) | 0.013(3) |
| C252 | 0.009(3) | 0.013(4) | 0.031(4) | 0.009(3) | 0.006(3) | 0.001(3) |
| C262 | 0.020(4) | 0.013(4) | 0.031(4) | 0.009(3) | 0.009(3) | 0.007(3) |
| C272 | 0.020(4) | 0.040(5) | 0.037(5) | 0.006(4) | | |

0.009(4)  0.019(4)
C282  0.028(5)  0.047(6)  0.038(5)  0.002(4)
0.015(4)  0.020(4)
C292  0.038(5)  0.033(5)  0.021(4)  0.002(4)
0.010(4)  0.015(4)
C302  0.018(4)  0.031(4)  0.031(5)  0.006(4)
0.005(3)  0.013(3)
C312  0.021(4)  0.023(4)  0.027(4)  0.009(3)
0.008(3)  0.015(3)
C322  0.019(4)  0.014(4)  0.025(4)  0.005(3)
0.005(3)  0.007(3)
C332  0.016(4)  0.020(4)  0.024(4)  0.009(3)
0.005(3)  0.010(3)
C342  0.019(4)  0.026(4)  0.024(4)  0.012(3)
0.002(3)  0.014(3)
C352  0.022(4)  0.016(4)  0.023(4)  0.011(3)
0.001(3)  -0.001(3)
C362  0.026(4)  0.033(5)  0.034(5)  0.019(4)
0.014(4)  0.018(4)
C372  0.018(4)  0.025(4)  0.033(4)  0.015(3)
0.012(3)  0.014(3)
C382  0.014(4)  0.009(3)  0.022(4)  0.003(3)
0.001(3)  0.004(3)
C392  0.008(3)  0.012(4)  0.027(4)  0.004(3)
0.002(3)  0.000(3)
C402  0.024(4)  0.019(4)  0.034(5)  0.007(3)
0.010(3)  0.009(3)
C412  0.031(5)  0.022(4)  0.045(5)  0.008(4)
0.019(4)  0.012(4)
C422  0.035(5)  0.025(4)  0.064(7)  0.014(4)
0.032(5)  0.021(4)
C432  0.025(4)  0.028(5)  0.063(6)  0.019(4)
0.011(4)  0.018(4)
C442  0.022(4)  0.023(4)  0.031(4)  0.011(3)
0.006(3)  0.011(3)
C452  0.022(4)  0.024(4)  0.032(4)  0.013(3)
0.006(3)  0.015(3)
C462  0.031(4)  0.016(4)  0.032(5)  0.005(3)
0.000(4)  0.007(3)
C472  0.040(5)  0.030(5)  0.043(6)  0.005(4)
-0.010(4)  0.012(4)
C482  0.069(7)  0.039(5)  0.027(5)  0.007(4)
0.008(5)  0.031(5)
C492  0.055(6)  0.036(5)  0.027(5)  0.008(4)
0.017(4)  0.025(5)
C502  0.033(5)  0.026(4)  0.034(5)  0.012(4)
0.020(4)  0.020(4)
Cl19  0.0733(19) 0.0611(17) 0.0494(16)  0.0057(13)
-0.0007(14)  0.0378(15)
C7  0.107(11)  0.053(7)  0.072(9)  0.022(6)
0.007(8)  0.030(7)
C6  0.066(7)  0.065(7)  0.094(9)  0.047(7)
0.029(7)  0.046(6)
Cl5  0.161(4) 0.0423(16)  0.068(2)  0.0292(15)
0.048(2)  0.0259(19)
Cl6  0.085(2) 0.0506(16) 0.0397(15) -0.0048(12)
0.0251(14) -0.0122(15)
C1  0.069(7)  0.037(6)  0.055(7)  0.016(5)
0.021(6)  0.004(5)
Cl7  0.078(2)  0.085(2) 0.0441(16) -0.0025(15)
0.0239(15) -0.0194(17)
Cl8  0.0652(19) 0.0669(19)  0.075(2)  0.0245(16)
0.0132(16)  0.0022(15)
C2  0.070(7)  0.057(7)  0.040(6)  -0.003(5)
0.021(5)  0.020(6)
Cl9  0.089(2)  0.081(2) 0.0662(18)  0.0394(16)
0.0358(16)  0.0584(18)

```
  Cl10      0.163(4)   0.097(3)   0.155(4)    0.091(3)
0.109(3)    0.096(3)
  C3        0.070(8)   0.088(9)   0.081(8)    0.058(7)
0.037(7)    0.048(7)
  Cl11    0.0676(17) 0.0501(15) 0.0372(13)  0.0151(11)
0.0161(12)  0.0132(13)
  Cl12      0.062(2)   0.052(2)   0.346(7)    0.071(3)
0.084(3)  0.0324(17)
  C4        0.056(7)   0.047(6)   0.059(7)    0.010(5)
0.023(5)    0.009(5)
  Cl13      0.100(4)   0.135(5)   0.328(9)    0.046(5)
0.105(5)    0.056(3)
  Cl14      0.086(3)   0.101(3)   0.342(8)    0.097(4)
0.066(4)    0.068(3)
  C5        0.043(8)  0.085(11)    0.37(3)   0.075(16)
0.060(14)    0.053(8)
  Cl2     0.0294(10)  0.0211(9) 0.0262(10)   0.0107(8)
0.0075(8)   0.0113(8)
  Cl3     0.0260(10) 0.0349(11) 0.0519(13)  0.0213(10)
0.0150(9)   0.0183(9)
  Cl4     0.0329(12) 0.0418(13) 0.0783(17)  0.0331(12)
0.0239(12)  0.0246(10)

#===============================================================

# 10. MOLECULAR GEOMETRY

_geom_special_details
;
 Bond distances, angles etc. have been calculated using the
 rounded fractional coordinates. All esds are estimated
 from the variances of the (full) variance-covariance matrix.
 The cell esds are taken into account in the estimation of
 distances, angles and torsion angles
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 Pd1     Cl1      2.8025(19)                    .       .
          yes
 Pd1     P1         2.243(2)                    .       .
          yes
 Pd1     P2         2.262(2)                    .       .
          yes
 Pd1     N1         2.086(6)                    .       .
          yes
 Pd1     N2         2.164(6)                    .       .
          yes
 P1      C381       1.811(8)                    .       .
          yes
 P1      C391       1.803(8)                    .       .
          yes
 P1      C451       1.810(8)                    .       .
          yes
 P2      C11        1.820(8)                    .       .
          yes
 P2      C71        1.824(6)                    .       .
          yes
 P2      C131       1.817(8)                    .       .
          yes
 N1      C191      1.281(10)                    .       .
          yes
```

| | | | | |
|---|---|---|---|---|
| N1 | C201 | 1.461(10) | . | . |
| | yes | | | |
| N2 | C311 | 1.452(10) | . | . |
| | yes | | | |
| N2 | C321 | 1.290(10) | . | . |
| | yes | | | |
| C11 | C21 | 1.397(11) | . | . |
| | no | | | |
| C11 | C61 | 1.379(11) | . | . |
| | no | | | |
| C21 | C31 | 1.405(12) | . | . |
| | no | | | |
| C31 | C41 | 1.375(14) | . | . |
| | no | | | |
| C41 | C51 | 1.375(14) | . | . |
| | no | | | |
| C51 | C61 | 1.385(13) | . | . |
| | no | | | |
| C71 | C81 | 1.387(10) | . | . |
| | no | | | |
| C71 | C121 | 1.387(11) | . | . |
| | no | | | |
| C81 | C91 | 1.363(11) | . | . |
| | no | | | |
| C91 | C101 | 1.382(13) | . | . |
| | no | | | |
| C101 | C111 | 1.371(12) | . | . |
| | no | | | |
| C111 | C121 | 1.391(11) | . | . |
| | no | | | |
| C131 | C141 | 1.413(10) | . | . |
| | no | | | |
| C131 | C181 | 1.409(11) | . | . |
| | no | | | |
| C141 | C151 | 1.382(11) | . | . |
| | no | | | |
| C151 | C161 | 1.390(11) | . | . |
| | no | | | |
| C161 | C171 | 1.387(11) | . | . |
| | no | | | |
| C171 | C181 | 1.399(11) | . | . |
| | no | | | |
| C181 | C191 | 1.445(11) | . | . |
| | no | | | |
| C201 | C211 | 1.384(11) | . | . |
| | no | | | |
| C201 | C251 | 1.390(11) | . | . |
| | no | | | |
| C211 | C221 | 1.395(13) | . | . |
| | no | | | |
| C221 | C231 | 1.369(13) | . | . |
| | no | | | |
| C231 | C241 | 1.369(11) | . | . |
| | no | | | |
| C241 | C251 | 1.393(11) | . | . |
| | no | | | |
| C251 | C261 | 1.470(11) | . | . |
| | no | | | |
| C261 | C271 | 1.382(12) | . | . |
| | no | | | |
| C261 | C311 | 1.409(11) | . | . |
| | no | | | |
| C271 | C281 | 1.375(11) | . | . |
| | no | | | |
| C281 | C291 | 1.389(11) | . | . |
| | no | | | |
| C291 | C301 | 1.386(11) | . | . |

| | | | | |
|---|---|---|---|---|
| | | no | | |
| C301 | C311 | 1.373(11) | . | . |
| | | no | | |
| C321 | C331 | 1.458(11) | . | . |
| | | no | | |
| C331 | C341 | 1.389(11) | . | . |
| | | no | | |
| C331 | C381 | 1.402(11) | . | . |
| | | no | | |
| C341 | C351 | 1.392(11) | . | . |
| | | no | | |
| C351 | C361 | 1.387(12) | . | . |
| | | no | | |
| C361 | C371 | 1.386(11) | . | . |
| | | no | | |
| C371 | C381 | 1.392(11) | . | . |
| | | no | | |
| C391 | C401 | 1.385(11) | . | . |
| | | no | | |
| C391 | C441 | 1.404(11) | . | . |
| | | no | | |
| C401 | C411 | 1.394(12) | . | . |
| | | no | | |
| C411 | C421 | 1.374(14) | . | . |
| | | no | | |
| C421 | C431 | 1.379(12) | . | . |
| | | no | | |
| C431 | C441 | 1.385(11) | . | . |
| | | no | | |
| C451 | C461 | 1.390(12) | . | . |
| | | no | | |
| C451 | C501 | 1.391(12) | . | . |
| | | no | | |
| C461 | C471 | 1.372(11) | . | . |
| | | no | | |
| C471 | C481 | 1.377(14) | . | . |
| | | no | | |
| C481 | C491 | 1.375(15) | . | . |
| | | no | | |
| C491 | C501 | 1.366(11) | . | . |
| | | no | | |
| C21 | H21 | 0.96(8) | . | . |
| | | no | | |
| C31 | H31 | 0.99(5) | . | . |
| | | no | | |
| C41 | H41 | 0.88(6) | . | . |
| | | no | | |
| C51 | H51 | 0.81(10) | . | . |
| | | no | | |
| C61 | H61 | 1.00(4) | . | . |
| | | no | | |
| C81 | H81 | 0.99(9) | . | . |
| | | no | | |
| C91 | H91 | 0.86(6) | . | . |
| | | no | | |
| C101 | H101 | 0.9293 | . | . |
| | | no | | |
| C111 | H111 | 0.95(9) | . | . |
| | | no | | |
| C121 | H121 | 0.79(5) | . | . |
| | | no | | |
| C141 | H141 | 0.92(6) | . | . |
| | | no | | |
| C151 | H151 | 1.01(7) | . | . |
| | | no | | |
| C161 | H161 | 0.96(6) | . | . |
| | | no | | |

| | | | | |
|---|---|---|---|---|
| C171 | H171 | 0.83(6) | . | . |
| | no | | | |
| C191 | H191 | 0.86(7) | . | . |
| | no | | | |
| C211 | H211 | 0.93(6) | . | . |
| | no | | | |
| C221 | H221 | 0.76(10) | . | . |
| | no | | | |
| C231 | H231 | 0.84(5) | . | . |
| | no | | | |
| C241 | H241 | 0.99(6) | . | . |
| | no | | | |
| C271 | H271 | 0.83(8) | . | . |
| | no | | | |
| C281 | H281 | 0.94(6) | . | . |
| | no | | | |
| C291 | H291 | 0.87(8) | . | . |
| | no | | | |
| C301 | H301 | 0.98(7) | . | . |
| | no | | | |
| C321 | H321 | 0.93(6) | . | . |
| | no | | | |
| C341 | H341 | 0.96(5) | . | . |
| | no | | | |
| C351 | H351 | 0.94(7) | . | . |
| | no | | | |
| C361 | H361 | 0.93(7) | . | . |
| | no | | | |
| C371 | H371 | 0.87(5) | . | . |
| | no | | | |
| C401 | H401 | 0.99(5) | . | . |
| | no | | | |
| C411 | H411 | 0.92(8) | . | . |
| | no | | | |
| C421 | H421 | 0.90(5) | . | . |
| | no | | | |
| C431 | H431 | 0.93(5) | . | . |
| | no | | | |
| C441 | H441 | 0.97(8) | . | . |
| | no | | | |
| C461 | H461 | 0.96(5) | . | . |
| | no | | | |
| C471 | H471 | 0.99(8) | . | . |
| | no | | | |
| C481 | H481 | 0.79(10) | . | . |
| | no | | | |
| C491 | H491 | 0.76(5) | . | . |
| | no | | | |
| C501 | H501 | 0.89(8) | . | . |
| | no | | | |
| Pd2 | P3 | 2.248(2) | . | . |
| | yes | | | |
| Pd2 | P4 | 2.271(2) | . | . |
| | yes | | | |
| Pd2 | N3 | 2.099(6) | . | . |
| | yes | | | |
| Pd2 | N4 | 2.166(6) | . | . |
| | yes | | | |
| P3 | C382 | 1.816(8) | . | . |
| | yes | | | |
| P3 | C392 | 1.796(8) | . | . |
| | yes | | | |
| P3 | C452 | 1.821(8) | . | . |
| | yes | | | |
| P4 | C12 | 1.818(8) | . | . |
| | yes | | | |
| P4 | C72 | 1.828(8) | . | . |

| | | | | |
|---|---|---|---|---|
| | yes | | | |
| P4 | C132 | 1.826(8) | . | . |
| | yes | | | |
| N3 | C192 | 1.248(10) | . | . |
| | yes | | | |
| N3 | C202 | 1.459(9) | . | . |
| | yes | | | |
| N4 | C312 | 1.468(10) | . | . |
| | yes | | | |
| N4 | C322 | 1.263(10) | . | . |
| | yes | | | |
| C12 | C22 | 1.396(11) | . | . |
| | no | | | |
| C12 | C62 | 1.389(11) | . | . |
| | no | | | |
| C22 | C32 | 1.392(12) | . | . |
| | no | | | |
| C32 | C42 | 1.377(12) | . | . |
| | no | | | |
| C42 | C52 | 1.369(14) | . | . |
| | no | | | |
| C52 | C62 | 1.387(13) | . | . |
| | no | | | |
| C72 | C82 | 1.374(11) | . | . |
| | no | | | |
| C72 | C122 | 1.404(11) | . | . |
| | no | | | |
| C82 | C92 | 1.377(11) | . | . |
| | no | | | |
| C92 | C102 | 1.377(13) | . | . |
| | no | | | |
| C102 | C112 | 1.397(12) | . | . |
| | no | | | |
| C112 | C122 | 1.367(11) | . | . |
| | no | | | |
| C132 | C142 | 1.399(11) | . | . |
| | no | | | |
| C132 | C182 | 1.387(11) | . | . |
| | no | | | |
| C142 | C152 | 1.397(13) | . | . |
| | no | | | |
| C152 | C162 | 1.374(14) | . | . |
| | no | | | |
| C162 | C172 | 1.381(12) | . | . |
| | no | | | |
| C172 | C182 | 1.390(11) | . | . |
| | no | | | |
| C182 | C192 | 1.462(11) | . | . |
| | no | | | |
| C202 | C212 | 1.373(10) | . | . |
| | no | | | |
| C202 | C252 | 1.398(10) | . | . |
| | no | | | |
| C212 | C222 | 1.381(12) | . | . |
| | no | | | |
| C222 | C232 | 1.396(13) | . | . |
| | no | | | |
| C232 | C242 | 1.377(11) | . | . |
| | no | | | |
| C242 | C252 | 1.396(11) | . | . |
| | no | | | |
| C252 | C262 | 1.475(11) | . | . |
| | no | | | |
| C262 | C272 | 1.397(12) | . | . |
| | no | | | |
| C262 | C312 | 1.387(11) | . | . |
| | no | | | |

| | | | | |
|---|---|---|---|---|
| C272 | C282 | 1.371(11) | . | . |
| | no | | | |
| C282 | C292 | 1.378(13) | . | . |
| | no | | | |
| C292 | C302 | 1.380(13) | . | . |
| | no | | | |
| C302 | C312 | 1.379(11) | . | . |
| | no | | | |
| C322 | C332 | 1.467(12) | . | . |
| | no | | | |
| C332 | C342 | 1.375(11) | . | . |
| | no | | | |
| C332 | C382 | 1.420(11) | . | . |
| | no | | | |
| C342 | C352 | 1.395(11) | . | . |
| | no | | | |
| C352 | C362 | 1.355(12) | . | . |
| | no | | | |
| C362 | C372 | 1.393(11) | . | . |
| | no | | | |
| C372 | C382 | 1.377(11) | . | . |
| | no | | | |
| C392 | C402 | 1.381(11) | . | . |
| | no | | | |
| C392 | C442 | 1.406(11) | . | . |
| | no | | | |
| C402 | C412 | 1.368(12) | . | . |
| | no | | | |
| C412 | C422 | 1.380(14) | . | . |
| | no | | | |
| C422 | C432 | 1.351(14) | . | . |
| | no | | | |
| C432 | C442 | 1.396(12) | . | . |
| | no | | | |
| C452 | C462 | 1.387(12) | . | . |
| | no | | | |
| C452 | C502 | 1.397(12) | . | . |
| | no | | | |
| C462 | C472 | 1.378(12) | . | . |
| | no | | | |
| C472 | C482 | 1.393(15) | . | . |
| | no | | | |
| C482 | C492 | 1.348(15) | . | . |
| | no | | | |
| C492 | C502 | 1.383(11) | . | . |
| | no | | | |
| C22 | H22 | 0.93(8) | . | . |
| | no | | | |
| C32 | H32 | 0.95(5) | . | . |
| | no | | | |
| C42 | H42 | 0.98(5) | . | . |
| | no | | | |
| C52 | H52 | 0.83(8) | . | . |
| | no | | | |
| C62 | H62 | 0.95(5) | . | . |
| | no | | | |
| C82 | H82 | 0.96(9) | . | . |
| | no | | | |
| C92 | H92 | 0.78(5) | . | . |
| | no | | | |
| C102 | H102 | 0.98(7) | . | . |
| | no | | | |
| C112 | H112 | 0.98(9) | . | . |
| | no | | | |
| C122 | H122 | 0.87(5) | . | . |
| | no | | | |
| C142 | H142 | 0.87(7) | . | . |

| | | | | |
|---|---|---|---|---|
| | | no | | |
| C152 | H152 | 0.92(7) | . | . |
| | | no | | |
| C162 | H162 | 0.91(7) | . | . |
| | | no | | |
| C172 | H172 | 0.98(6) | . | . |
| | | no | | |
| C192 | H192 | 0.94(7) | . | . |
| | | no | | |
| C212 | H212 | 0.92(6) | . | . |
| | | no | | |
| C222 | H222 | 0.98(8) | . | . |
| | | no | | |
| C232 | H232 | 0.80(5) | . | . |
| | | no | | |
| C242 | H242 | 0.98(6) | . | . |
| | | no | | |
| C272 | H272 | 0.82(8) | . | . |
| | | no | | |
| C282 | H282 | 0.97(6) | . | . |
| | | no | | |
| C292 | H292 | 0.85(8) | . | . |
| | | no | | |
| C302 | H302 | 0.89(7) | . | . |
| | | no | | |
| C322 | H322 | 0.92(6) | . | . |
| | | no | | |
| C342 | H342 | 0.81(5) | . | . |
| | | no | | |
| C352 | H352 | 0.87(7) | . | . |
| | | no | | |
| C362 | H362 | 0.93(7) | . | . |
| | | no | | |
| C372 | H372 | 0.98(5) | . | . |
| | | no | | |
| C402 | H402 | 0.79(6) | . | . |
| | | no | | |
| C412 | H412 | 0.94(8) | . | . |
| | | no | | |
| C422 | H422 | 0.95(5) | . | . |
| | | no | | |
| C432 | H432 | 0.85(6) | . | . |
| | | no | | |
| C442 | H442 | 1.00(8) | . | . |
| | | no | | |
| C462 | H462 | 0.93(5) | . | . |
| | | no | | |
| C472 | H472 | 0.93(8) | . | . |
| | | no | | |
| C482 | H482 | 1.00(10) | . | . |
| | | no | | |
| C492 | H492 | 0.87(6) | . | . |
| | | no | | |
| C502 | H502 | 0.90(8) | . | . |
| | | no | | |
| Cl19 | C7 | 1.762(13) | . | . |
| | | yes | | |
| Cl20 | C7 | 1.74(2) | . | . |
| | | yes | | |
| Cl21 | C7 | 1.78(4) | . | . |
| | | yes | | |
| Cl22 | C7 | 1.68(2) | . | . |
| | | yes | | |
| C7 | H310 | 0.9710 | . | . |
| | | no | | |
| C7 | H320 | 0.9691 | . | . |
| | | no | | |

```
 C7      H330         0.9710                    .       .
          no
 C7      H340         0.9700                    .       .
          no
 C7      H350         0.9698                    .       .
          no
 C7      H360         0.9689                    .       .
          no
 Cl15    C6        1.807(13)                    .       .
          yes
 Cl16    C6        1.641(14)                    .       .
          yes
 Cl17    C6          1.77(2)                    .       .
          yes
 Cl18    C6        1.552(16)                    .       .
          yes
 C6      H610         0.9703                    .       .
          no
 C6      H620         0.9698                    .       .
          no
 C6      H630         0.9702                    .       .
          no
 C6      H640         0.9699                    .       .
          no
 Cl5     C1        1.717(10)                    .       .
          yes
 Cl6     C1        1.747(12)                    .       .
          yes
 C1      H11          0.9709                    .       .
          no
 C1      H201         0.9706                    .       .
          no
 Cl7     C2        1.757(12)                    .       .
          yes
 Cl8     C2        1.731(13)                    .       .
          yes
 C2      H12          0.9704                    .       .
          no
 C2      H202         0.9688                    .       .
          no
 Cl9     C3        1.765(13)                    .       .
          yes
 Cl10    C3        1.749(14)                    .       .
          yes
 C3      H13          0.9695                    .       .
          no
 C3      H203         0.9708                    .       .
          no
 Cl11    C4        1.736(11)                    .       .
          yes
 Cl12    C4        1.727(11)                    .       .
          yes
 C4      H14          0.9709                    .       .
          no
 C4      H204         0.9706                    .       .
          no
 Cl13    C5          1.73(3)                    .       .
          yes
 Cl14    C5          1.71(2)                    .       .
          yes
 C5      H15          0.9701                    .       .
          no
 C5      H205         0.9707                    .       .
          no

loop_
_geom_angle_atom_site_label_1
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_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
 Cl1     Pd1     P1         86.86(7)             .       .
.           yes
 Cl1     Pd1     P2        112.39(6)             .       .
.           yes
 Cl1     Pd1     N1         92.08(17)            .       .
.           yes
 Cl1     Pd1     N2         85.59(16)            .       .
.           yes
 P1      Pd1     P2         96.56(8)             .       .
.           yes
 P1      Pd1     N1        175.08(17)            .       .
.           yes
 P1      Pd1     N2         85.08(18)            .       .
.           yes
 P2      Pd1     N1         88.29(17)            .       .
.           yes
 P2      Pd1     N2        161.98(16)            .       .
.           yes
 N1      Pd1     N2           90.0(2)            .       .
.           yes
 Pd1     P1      C381       108.2(3)             .       .
.           yes
 Pd1     P1      C391       117.4(3)             .       .
.           yes
 Pd1     P1      C451       113.0(3)             .       .
.           yes
 C381    P1      C391       103.1(4)             .       .
.           yes
 C381    P1      C451       104.6(3)             .       .
.           yes
 C391    P1      C451       109.4(4)             .       .
.           yes
 Pd1     P2      C11        119.3(3)             .       .
.           yes
 Pd1     P2      C71        115.2(2)             .       .
.           yes
 Pd1     P2      C131       108.8(3)             .       .
.           yes
 C11     P2      C71        106.4(4)             .       .
.           yes
 C11     P2      C131       102.2(3)             .       .
.           yes
 C71     P2      C131       103.1(3)             .       .
.           yes
 Pd1     N1      C191       130.8(5)             .       .
.           yes
 Pd1     N1      C201       115.9(5)             .       .
.           yes
 C191    N1      C201       113.3(7)             .       .
.           yes
 Pd1     N2      C311       117.0(4)             .       .
.           yes
 Pd1     N2      C321       128.4(5)             .       .
.           yes
 C311    N2      C321       114.6(6)             .       .
.           yes
 P2      C11     C21        122.6(6)             .       .
.           yes
 P2      C11     C61        119.3(6)             .       .
.           yes
```

| | | | | | |
|---|---|---|---|---|---|
| C21 | C11 | C61 | 118.1(7) | . | . |
| . | no | | | | |
| C11 | C21 | C31 | 120.5(7) | . | . |
| . | no | | | | |
| C21 | C31 | C41 | 119.2(8) | . | . |
| . | no | | | | |
| C31 | C41 | C51 | 121.0(9) | . | . |
| . | no | | | | |
| C41 | C51 | C61 | 119.3(9) | . | . |
| . | no | | | | |
| C11 | C61 | C51 | 121.8(8) | . | . |
| . | no | | | | |
| P2 | C71 | C81 | 120.0(6) | . | . |
| . | yes | | | | |
| P2 | C71 | C121 | 119.8(5) | . | . |
| . | yes | | | | |
| C81 | C71 | C121 | 120.1(6) | . | . |
| . | no | | | | |
| C71 | C81 | C91 | 119.1(7) | . | . |
| . | no | | | | |
| C81 | C91 | C101 | 121.7(8) | . | . |
| . | no | | | | |
| C91 | C101 | C111 | 119.2(7) | . | . |
| . | no | | | | |
| C101 | C111 | C121 | 120.2(8) | . | . |
| . | no | | | | |
| C71 | C121 | C111 | 119.5(7) | . | . |
| . | no | | | | |
| P2 | C131 | C141 | 119.6(6) | . | . |
| . | yes | | | | |
| P2 | C131 | C181 | 122.5(6) | . | . |
| . | yes | | | | |
| C141 | C131 | C181 | 117.8(7) | . | . |
| . | no | | | | |
| C131 | C141 | C151 | 121.8(7) | . | . |
| . | no | | | | |
| C141 | C151 | C161 | 119.6(7) | . | . |
| . | no | | | | |
| C151 | C161 | C171 | 120.0(7) | . | . |
| . | no | | | | |
| C161 | C171 | C181 | 120.8(7) | . | . |
| . | no | | | | |
| C131 | C181 | C171 | 120.0(7) | . | . |
| . | no | | | | |
| C131 | C181 | C191 | 125.3(7) | . | . |
| . | no | | | | |
| C171 | C181 | C191 | 114.6(7) | . | . |
| . | no | | | | |
| N1 | C191 | C181 | 127.7(7) | . | . |
| . | yes | | | | |
| N1 | C201 | C211 | 118.5(7) | . | . |
| . | yes | | | | |
| N1 | C201 | C251 | 119.5(7) | . | . |
| . | yes | | | | |
| C211 | C201 | C251 | 121.7(7) | . | . |
| . | no | | | | |
| C201 | C211 | C221 | 118.2(8) | . | . |
| . | no | | | | |
| C211 | C221 | C231 | 121.1(7) | . | . |
| . | no | | | | |
| C221 | C231 | C241 | 119.7(8) | . | . |
| . | no | | | | |
| C231 | C241 | C251 | 121.5(8) | . | . |
| . | no | | | | |
| C201 | C251 | C241 | 117.8(7) | . | . |
| . | no | | | | |
| C201 | C251 | C261 | 122.6(7) | . | . |

```
.           no
 C241    C251    C261       119.5(7)            .       .
.           no
 C251    C261    C271       120.5(7)            .       .
.           no
 C251    C261    C311       122.5(7)            .       .
.           no
 C271    C261    C311       116.8(7)            .       .
.           no
 C261    C271    C281       122.7(8)            .       .
.           no
 C271    C281    C291       119.3(8)            .       .
.           no
 C281    C291    C301       119.6(7)            .       .
.           no
 C291    C301    C311       120.2(8)            .       .
.           no
 N2      C311    C261       121.0(7)            .       .
.           yes
 N2      C311    C301       117.5(7)            .       .
.           yes
 C261    C311    C301       121.3(7)            .       .
.           no
 N2      C321    C331       127.5(7)            .       .
.           yes
 C321    C331    C341       115.5(7)            .       .
.           no
 C321    C331    C381       123.9(7)            .       .
.           no
 C341    C331    C381       120.6(7)            .       .
.           no
 C331    C341    C351       120.7(7)            .       .
.           no
 C341    C351    C361       119.2(7)            .       .
.           no
 C351    C361    C371       119.7(8)            .       .
.           no
 C361    C371    C381       122.1(8)            .       .
.           no
 P1      C381    C331       121.7(6)            .       .
.           yes
 P1      C381    C371       120.6(6)            .       .
.           yes
 C331    C381    C371       117.6(7)            .       .
.           no
 P1      C391    C401       116.7(6)            .       .
.           yes
 P1      C391    C441       123.1(6)            .       .
.           yes
 C401    C391    C441       120.1(7)            .       .
.           no
 C391    C401    C411       119.7(8)            .       .
.           no
 C401    C411    C421       120.1(9)            .       .
.           no
 C411    C421    C431       120.3(9)            .       .
.           no
 C421    C431    C441       120.7(8)            .       .
.           no
 C391    C441    C431       119.0(7)            .       .
.           no
 P1      C451    C461       121.3(6)            .       .
.           yes
 P1      C451    C501       120.2(6)            .       .
.           yes
 C461    C451    C501       118.5(7)            .       .
.           no
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 C451    C461    C471       120.7(8)            .       .
.           no
 C461    C471    C481       119.3(9)            .       .
.           no
 C471    C481    C491       121.1(8)            .       .
.           no
 C481    C491    C501       119.3(9)            .       .
.           no
 C451    C501    C491       121.1(9)            .       .
.           no
 C11     C21     H21       119.7(17)            .       .
.           no
 C31     C21     H21       119.8(17)            .       .
.           no
 C21     C31     H31          121(2)            .       .
.           no
 C41     C31     H31          120(2)            .       .
.           no
 C31     C41     H41          119(4)            .       .
.           no
 C51     C41     H41          120(4)            .       .
.           no
 C41     C51     H51          120(3)            .       .
.           no
 C61     C51     H51          120(3)            .       .
.           no
 C11     C61     H61          119(2)            .       .
.           no
 C51     C61     H61          119(2)            .       .
.           no
 C71     C81     H81       120.6(19)            .       .
.           no
 C91     C81     H81       120.3(19)            .       .
.           no
 C81     C91     H91          119(4)            .       .
.           no
 C101    C91     H91          119(4)            .       .
.           no
 C91     C101    H101         120.45            .       .
.           no
 C111    C101    H101         120.32            .       .
.           no
 C101    C111    H111         120(2)            .       .
.           no
 C121    C111    H111         120(2)            .       .
.           no
 C71     C121    H121         121(4)            .       .
.           no
 C111    C121    H121         120(4)            .       .
.           no
 C131    C141    H141         119(2)            .       .
.           no
 C151    C141    H141         119(2)            .       .
.           no
 C141    C151    H151         120(2)            .       .
.           no
 C161    C151    H151         120(2)            .       .
.           no
 C151    C161    H161         119(3)            .       .
.           no
 C171    C161    H161         121(3)            .       .
.           no
 C161    C171    H171         120(2)            .       .
.           no
 C181    C171    H171         120(2)            .       .
.           no
 N1      C191    H191      116.1(14)            .       .
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.           no
 C181    C191    H191      116.2(14)            .       .
.           no
 C201    C211    H211         121(3)            .       .
.           no
 C221    C211    H211         121(3)            .       .
.           no
 C211    C221    H221         120(3)            .       .
.           no
 C231    C221    H221         119(3)            .       .
.           no
 C221    C231    H231         120(3)            .       .
.           no
 C241    C231    H231         121(3)            .       .
.           no
 C231    C241    H241         119(3)            .       .
.           no
 C251    C241    H241         119(3)            .       .
.           no
 C261    C271    H271         119(4)            .       .
.           no
 C281    C271    H271         119(4)            .       .
.           no
 C271    C281    H281         120(3)            .       .
.           no
 C291    C281    H281         120(3)            .       .
.           no
 C281    C291    H291         120(2)            .       .
.           no
 C301    C291    H291         120(2)            .       .
.           no
 C291    C301    H301         120(3)            .       .
.           no
 C311    C301    H301         120(3)            .       .
.           no
 N2      C321    H321         116(3)            .       .
.           no
 C331    C321    H321         116(3)            .       .
.           no
 C331    C341    H341         120(3)            .       .
.           no
 C351    C341    H341         120(3)            .       .
.           no
 C341    C351    H351         121(3)            .       .
.           no
 C361    C351    H351         120(3)            .       .
.           no
 C351    C361    H361      120.3(19)            .       .
.           no
 C371    C361    H361      119.9(19)            .       .
.           no
 C361    C371    H371         119(3)            .       .
.           no
 C381    C371    H371         119(3)            .       .
.           no
 C391    C401    H401         120(3)            .       .
.           no
 C411    C401    H401         120(3)            .       .
.           no
 C401    C411    H411      120.0(19)            .       .
.           no
 C421    C411    H411         120(2)            .       .
.           no
 C411    C421    H421         120(3)            .       .
.           no
 C431    C421    H421         119(3)            .       .
.           no
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 C421    C431    H431         119(3)             .       .
.           no
 C441    C431    H431         120(3)             .       .
.           no
 C391    C441    H441      120.5(17)             .       .
.           no
 C431    C441    H441      120.5(17)             .       .
.           no
 C451    C461    H461         119(3)             .       .
.           no
 C471    C461    H461         120(3)             .       .
.           no
 C461    C471    H471         120(3)             .       .
.           no
 C481    C471    H471         121(3)             .       .
.           no
 C471    C481    H481         119(3)             .       .
.           no
 C491    C481    H481         120(3)             .       .
.           no
 C481    C491    H491         121(4)             .       .
.           no
 C501    C491    H491         120(4)             .       .
.           no
 C451    C501    H501         120(3)             .       .
.           no
 C491    C501    H501         119(3)             .       .
.           no
 P3      Pd2     P4          97.19(8)            .       .
.           yes
 P3      Pd2     N3       174.79(16)             .       .
.           yes
 P3      Pd2     N4        84.04(18)             .       .
.           yes
 P4      Pd2     N3        87.93(17)             .       .
.           yes
 P4      Pd2     N4       164.41(16)             .       .
.           yes
 N3      Pd2     N4          90.8(2)             .       .
.           yes
 Pd2     P3      C382       108.0(3)             .       .
.           yes
 Pd2     P3      C392       120.1(3)             .       .
.           yes
 Pd2     P3      C452       113.2(3)             .       .
.           yes
 C382    P3      C392       102.3(4)             .       .
.           yes
 C382    P3      C452       102.9(3)             .       .
.           yes
 C392    P3      C452       108.5(4)             .       .
.           yes
 Pd2     P4      C12        118.3(3)             .       .
.           yes
 Pd2     P4      C72        116.3(3)             .       .
.           yes
 Pd2     P4      C132       108.7(3)             .       .
.           yes
 C12     P4      C72        105.6(4)             .       .
.           yes
 C12     P4      C132       103.2(4)             .       .
.           yes
 C72     P4      C132       102.9(4)             .       .
.           yes
 Pd2     N3      C192       131.0(5)             .       .
.           yes
 Pd2     N3      C202       115.5(5)             .       .
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.           yes
 C192    N3      C202       113.4(7)            .       .
.           yes
 Pd2     N4      C312       115.9(4)            .       .
.           yes
 Pd2     N4      C322       129.2(5)            .       .
.           yes
 C312    N4      C322       114.8(6)            .       .
.           yes
 P4      C12     C22        121.6(6)            .       .
.           yes
 P4      C12     C62        119.3(6)            .       .
.           yes
 C22     C12     C62        119.1(7)            .       .
.           no
 C12     C22     C32        119.9(7)            .       .
.           no
 C22     C32     C42        120.2(8)            .       .
.           no
 C32     C42     C52        120.1(9)            .       .
.           no
 C42     C52     C62        120.7(8)            .       .
.           no
 C12     C62     C52        120.0(8)            .       .
.           no
 P4      C72     C82        122.0(6)            .       .
.           yes
 P4      C72     C122       118.5(6)            .       .
.           yes
 C82     C72     C122       119.5(7)            .       .
.           no
 C72     C82     C92        120.1(7)            .       .
.           no
 C82     C92     C102       120.8(8)            .       .
.           no
 C92     C102    C112       119.2(7)            .       .
.           no
 C102    C112    C122       120.3(8)            .       .
.           no
 C72     C122    C112       120.0(7)            .       .
.           no
 P4      C132    C142       118.4(6)            .       .
.           yes
 P4      C132    C182       122.1(6)            .       .
.           yes
 C142    C132    C182       119.2(8)            .       .
.           no
 C132    C142    C152       120.1(8)            .       .
.           no
 C142    C152    C162       120.4(8)            .       .
.           no
 C152    C162    C172       119.4(9)            .       .
.           no
 C162    C172    C182       121.1(8)            .       .
.           no
 C132    C182    C172       119.8(7)            .       .
.           no
 C132    C182    C192       124.7(7)            .       .
.           no
 C172    C182    C192       115.5(7)            .       .
.           no
 N3      C192    C182       129.1(8)            .       .
.           yes
 N3      C202    C212       119.2(6)            .       .
.           yes
 N3      C202    C252       119.5(6)            .       .
.           yes
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 C212    C202    C252       121.2(7)            .       .
.           no
 C202    C212    C222       121.3(7)            .       .
.           no
 C212    C222    C232       118.2(7)            .       .
.           no
 C222    C232    C242       120.6(8)            .       .
.           no
 C232    C242    C252       121.3(7)            .       .
.           no
 C202    C252    C242       117.3(7)            .       .
.           no
 C202    C252    C262       122.4(7)            .       .
.           no
 C242    C252    C262       120.0(7)            .       .
.           no
 C252    C262    C272       119.6(7)            .       .
.           no
 C252    C262    C312       123.7(7)            .       .
.           no
 C272    C262    C312       116.6(7)            .       .
.           no
 C262    C272    C282       122.2(9)            .       .
.           no
 C272    C282    C292       119.1(9)            .       .
.           no
 C282    C292    C302       120.8(7)            .       .
.           no
 C292    C302    C312       118.9(8)            .       .
.           no
 N4      C312    C262       119.8(7)            .       .
.           yes
 N4      C312    C302       117.7(7)            .       .
.           yes
 C262    C312    C302       122.3(8)            .       .
.           no
 N4      C322    C332       128.2(7)            .       .
.           yes
 C322    C332    C342       116.5(7)            .       .
.           no
 C322    C332    C382       123.5(7)            .       .
.           no
 C342    C332    C382       120.0(7)            .       .
.           no
 C332    C342    C352       120.1(7)            .       .
.           no
 C342    C352    C362       120.3(7)            .       .
.           no
 C352    C362    C372       120.4(8)            .       .
.           no
 C362    C372    C382       120.8(8)            .       .
.           no
 P3      C382    C332       119.8(6)            .       .
.           yes
 P3      C382    C372       121.5(6)            .       .
.           yes
 C332    C382    C372       118.4(7)            .       .
.           no
 P3      C392    C402       118.1(6)            .       .
.           yes
 P3      C392    C442       122.5(6)            .       .
.           yes
 C402    C392    C442       119.4(7)            .       .
.           no
 C392    C402    C412       121.2(8)            .       .
.           no
 C402    C412    C422       119.4(9)            .       .
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```
.           no
 C412    C422    C432       120.6(9)            .       .
.           no
 C422    C432    C442       121.4(9)            .       .
.           no
 C392    C442    C432       118.0(7)            .       .
.           no
 P3      C452    C462       120.9(6)            .       .
.           yes
 P3      C452    C502       119.4(6)            .       .
.           yes
 C462    C452    C502       119.8(7)            .       .
.           no
 C452    C462    C472       119.5(8)            .       .
.           no
 C462    C472    C482       119.7(9)            .       .
.           no
 C472    C482    C492       121.3(9)            .       .
.           no
 C482    C492    C502       119.8(9)            .       .
.           no
 C452    C502    C492       120.0(8)            .       .
.           no
 C12     C22     H22          120(2)            .       .
.           no
 C32     C22     H22          120(2)            .       .
.           no
 C22     C32     H32          120(3)            .       .
.           no
 C42     C32     H32          120(3)            .       .
.           no
 C32     C42     H42          120(3)            .       .
.           no
 C52     C42     H42          120(3)            .       .
.           no
 C42     C52     H52          120(2)            .       .
.           no
 C62     C52     H52          120(2)            .       .
.           no
 C12     C62     H62          120(3)            .       .
.           no
 C52     C62     H62          120(3)            .       .
.           no
 C72     C82     H82       120.0(18)            .       .
.           no
 C92     C82     H82       119.9(18)            .       .
.           no
 C82     C92     H92          120(4)            .       .
.           no
 C102    C92     H92          119(4)            .       .
.           no
 C92     C102    H102         120(4)            .       .
.           no
 C112    C102    H102         120(4)            .       .
.           no
 C102    C112    H112      120.0(18)            .       .
.           no
 C122    C112    H112      119.8(18)            .       .
.           no
 C72     C122    H122         120(3)            .       .
.           no
 C112    C122    H122         120(3)            .       .
.           no
 C132    C142    H142         120(3)            .       .
.           no
 C152    C142    H142         120(3)            .       .
.           no
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| | | | | | |
|---|---|---|---|---|---|
| C142 | C152 | H152 | 120(2) | . | . |
| . | no | | | | |
| C162 | C152 | H152 | 120(2) | . | . |
| . | no | | | | |
| C152 | C162 | H162 | 120(4) | . | . |
| . | no | | | | |
| C172 | C162 | H162 | 120(4) | . | . |
| . | no | | | | |
| C162 | C172 | H172 | 119.5(19) | . | . |
| . | no | | | | |
| C182 | C172 | H172 | 119.4(19) | . | . |
| . | no | | | | |
| N3 | C192 | H192 | 115.5(14) | . | . |
| . | no | | | | |
| C182 | C192 | H192 | 115.5(13) | . | . |
| . | no | | | | |
| C202 | C212 | H212 | 120(3) | . | . |
| . | no | | | | |
| C222 | C212 | H212 | 119(3) | . | . |
| . | no | | | | |
| C212 | C222 | H222 | 121(2) | . | . |
| . | no | | | | |
| C232 | C222 | H222 | 121(2) | . | . |
| . | no | | | | |
| C222 | C232 | H232 | 120(3) | . | . |
| . | no | | | | |
| C242 | C232 | H232 | 120(3) | . | . |
| . | no | | | | |
| C232 | C242 | H242 | 120(3) | . | . |
| . | no | | | | |
| C252 | C242 | H242 | 119(3) | . | . |
| . | no | | | | |
| C262 | C272 | H272 | 119(4) | . | . |
| . | no | | | | |
| C282 | C272 | H272 | 119(4) | . | . |
| . | no | | | | |
| C272 | C282 | H282 | 120(3) | . | . |
| . | no | | | | |
| C292 | C282 | H282 | 120(3) | . | . |
| . | no | | | | |
| C282 | C292 | H292 | 119(3) | . | . |
| . | no | | | | |
| C302 | C292 | H292 | 120(3) | . | . |
| . | no | | | | |
| C292 | C302 | H302 | 120(3) | . | . |
| . | no | | | | |
| C312 | C302 | H302 | 121(3) | . | . |
| . | no | | | | |
| N4 | C322 | H322 | 116(3) | . | . |
| . | no | | | | |
| C332 | C322 | H322 | 116(3) | . | . |
| . | no | | | | |
| C332 | C342 | H342 | 120(3) | . | . |
| . | no | | | | |
| C352 | C342 | H342 | 120(3) | . | . |
| . | no | | | | |
| C342 | C352 | H352 | 120(4) | . | . |
| . | no | | | | |
| C362 | C352 | H352 | 119(4) | . | . |
| . | no | | | | |
| C352 | C362 | H362 | 119.9(18) | . | . |
| . | no | | | | |
| C372 | C362 | H362 | 119.8(19) | . | . |
| . | no | | | | |
| C362 | C372 | H372 | 120(3) | . | . |
| . | no | | | | |
| C382 | C372 | H372 | 119(3) | . | . |

```
.          no
 C392    C402    H402         120(4)            .       .
.          no
 C412    C402    H402         119(4)            .       .
.          no
 C402    C412    H412         120(2)            .       .
.          no
 C422    C412    H412         120(2)            .       .
.          no
 C412    C422    H422         120(2)            .       .
.          no
 C432    C422    H422         120(2)            .       .
.          no
 C422    C432    H432         119(4)            .       .
.          no
 C442    C432    H432         120(4)            .       .
.          no
 C392    C442    H442      121.0(19)            .       .
.          no
 C432    C442    H442      121.0(19)            .       .
.          no
 C452    C462    H462         120(3)            .       .
.          no
 C472    C462    H462         120(3)            .       .
.          no
 C462    C472    H472         120(3)            .       .
.          no
 C482    C472    H472         120(3)            .       .
.          no
 C472    C482    H482         119(3)            .       .
.          no
 C492    C482    H482         119(2)            .       .
.          no
 C482    C492    H492         120(4)            .       .
.          no
 C502    C492    H492         120(4)            .       .
.          no
 C452    C502    H502         120(3)            .       .
.          no
 C492    C502    H502         120(3)            .       .
.          no
 Cl19    C7      Cl20          118.6(9)         .       .
.          yes
 Cl19    C7      Cl21      100.5(14)            .       .
.          yes
 Cl19    C7      Cl22      105.8(13)            .       .
.          yes
 Cl19    C7      H310         107.68            .       .
.          no
 Cl19    C7      H320         107.76            .       .
.          no
 Cl19    C7      H330         111.67            .       .
.          no
 Cl19    C7      H340         111.71            .       .
.          no
 Cl19    C7      H350         110.58            .       .
.          no
 Cl19    C7      H360         110.63            .       .
.          no
 Cl20    C7      H310         107.64            .       .
.          no
 Cl20    C7      H320         107.57            .       .
.          no
 H310    C7      H320         107.12            .       .
.          no
 Cl21    C7      H330         111.58            .       .
.          no
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 Cl21    C7      H340         111.64             .       .
.            no
 Cl22    C7      H350         110.49             .       .
.            no
 Cl22    C7      H360         110.60             .       .
.            no
 H330    C7      H340         109.57             .       .
.            no
 H350    C7      H360         108.71             .       .
.            no
 Cl15    C6      Cl16        111.6(7)            .       .
.            yes
 Cl17    C6      Cl18       120.8(12)            .       .
.            yes
 Cl15    C6      H610         109.27             .       .
.            no
 Cl15    C6      H620         109.24             .       .
.            no
 Cl16    C6      H610         109.34             .       .
.            no
 Cl16    C6      H620         109.32             .       .
.            no
 H610    C6      H620         108.05             .       .
.            no
 Cl17    C6      H630         107.22             .       .
.            no
 Cl17    C6      H640         107.15             .       .
.            no
 Cl18    C6      H630         107.05             .       .
.            no
 Cl18    C6      H640         107.13             .       .
.            no
 H630    C6      H640         106.77             .       .
.            no
 Cl5     C1      Cl6         113.3(7)            .       .
.            yes
 Cl5     C1      H11          108.94             .       .
.            no
 Cl5     C1      H201         108.99             .       .
.            no
 Cl6     C1      H11          108.85             .       .
.            no
 Cl6     C1      H201         108.92             .       .
.            no
 H11     C1      H201         107.72             .       .
.            no
 Cl7     C2      Cl8         111.4(6)            .       .
.            yes
 Cl7     C2      H12          109.32             .       .
.            no
 Cl7     C2      H202         109.39             .       .
.            no
 Cl8     C2      H12          109.33             .       .
.            no
 Cl8     C2      H202         109.40             .       .
.            no
 H12     C2      H202         107.97             .       .
.            no
 Cl9     C3      Cl10        110.6(7)            .       .
.            yes
 Cl9     C3      H13          109.60             .       .
.            no
 Cl9     C3      H203         109.43             .       .
.            no
 Cl10    C3      H13          109.56             .       .
.            no
 Cl10    C3      H203         109.46             .       .
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.          no
 H13    C3      H203         108.10            .       .
.          no
 Cl11   C4      Cl12        111.5(7)           .       .
.          yes
 Cl11   C4      H14          109.35            .       .
.          no
 Cl11   C4      H204         109.30            .       .
.          no
 Cl12   C4      H14          109.32            .       .
.          no
 Cl12   C4      H204         109.43            .       .
.          no
 H14    C4      H204         107.87            .       .
.          no
 Cl13   C5      Cl14       113.4(11)           .       .
.          yes
 Cl13   C5      H15          108.94            .       .
.          no
 Cl13   C5      H205         108.87            .       .
.          no
 Cl14   C5      H15          108.86            .       .
.          no
 Cl14   C5      H205         108.95            .       .
.          no
 H15    C5      H205         107.71            .       .
.          no

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag
 Cl1    Pd1     P1      C381       -39.4(2)     .       .
.       .   no
 Cl1    Pd1     P1      C391        76.6(3)     .       .
.       .   no
 Cl1    Pd1     P1      C451      -154.7(3)     .       .
.       .   no
 P2     Pd1     P1      C381      -151.6(2)     .       .
.       .   no
 P2     Pd1     P1      C391       -35.6(3)     .       .
.       .   no
 P2     Pd1     P1      C451        93.1(3)     .       .
.       .   no
 N2     Pd1     P1      C381        46.4(3)     .       .
.       .   no
 N2     Pd1     P1      C391       162.4(3)     .       .
.       .   no
 N2     Pd1     P1      C451       -68.9(3)     .       .
.       .   no
 Cl1    Pd1     P2      C11       -114.0(3)     .       .
.       .   no
 Cl1    Pd1     P2      C71         14.4(3)     .       .
.       .   no
 Cl1    Pd1     P2      C131       129.6(2)     .       .
.       .   no
 P1     Pd1     P2      C11        -24.7(3)     .       .
.       .   no
 P1     Pd1     P2      C71        103.7(3)     .       .
.       .   no
```

| | | | | | | |
|---|---|---|---|---|---|---|
| P1 | Pd1 | P2 | C131 | -141.1(2) | . | . |
| . | . | no | | | | |
| N1 | Pd1 | P2 | C11 | 154.5(3) | . | . |
| . | . | no | | | | |
| N1 | Pd1 | P2 | C71 | -77.1(3) | . | . |
| . | . | no | | | | |
| N1 | Pd1 | P2 | C131 | 38.0(3) | . | . |
| . | . | no | | | | |
| Cl1 | Pd1 | N1 | C191 | -144.3(7) | . | . |
| . | . | no | | | | |
| Cl1 | Pd1 | N1 | C201 | 37.7(5) | . | . |
| . | . | no | | | | |
| P2 | Pd1 | N1 | C191 | -32.0(7) | . | . |
| . | . | no | | | | |
| P2 | Pd1 | N1 | C201 | 150.1(5) | . | . |
| . | . | no | | | | |
| N2 | Pd1 | N1 | C191 | 130.1(7) | . | . |
| . | . | no | | | | |
| N2 | Pd1 | N1 | C201 | -47.9(5) | . | . |
| . | . | no | | | | |
| Cl1 | Pd1 | N2 | C311 | -134.0(5) | . | . |
| . | . | no | | | | |
| Cl1 | Pd1 | N2 | C321 | 49.1(6) | . | . |
| . | . | no | | | | |
| P1 | Pd1 | N2 | C311 | 138.8(5) | . | . |
| . | . | no | | | | |
| P1 | Pd1 | N2 | C321 | -38.1(6) | . | . |
| . | . | no | | | | |
| N1 | Pd1 | N2 | C311 | -41.9(5) | . | . |
| . | . | no | | | | |
| N1 | Pd1 | N2 | C321 | 141.2(6) | . | . |
| . | . | no | | | | |
| C451 | P1 | C391 | C441 | 2.1(8) | . | . |
| . | . | no | | | | |
| C391 | P1 | C381 | C371 | 15.3(6) | . | . |
| . | . | no | | | | |
| C451 | P1 | C381 | C371 | -99.0(6) | . | . |
| . | . | no | | | | |
| Pd1 | P1 | C391 | C401 | -51.6(7) | . | . |
| . | . | no | | | | |
| Pd1 | P1 | C381 | C331 | -41.6(6) | . | . |
| . | . | no | | | | |
| C391 | P1 | C381 | C331 | -166.6(6) | . | . |
| . | . | no | | | | |
| C451 | P1 | C381 | C331 | 79.1(6) | . | . |
| . | . | no | | | | |
| Pd1 | P1 | C381 | C371 | 140.4(5) | . | . |
| . | . | no | | | | |
| C391 | P1 | C451 | C501 | 124.7(7) | . | . |
| . | . | no | | | | |
| C451 | P1 | C391 | C401 | 178.0(6) | . | . |
| . | . | no | | | | |
| Pd1 | P1 | C451 | C461 | 170.8(6) | . | . |
| . | . | no | | | | |
| C381 | P1 | C391 | C401 | 67.1(7) | . | . |
| . | . | no | | | | |
| C381 | P1 | C451 | C461 | 53.4(7) | . | . |
| . | . | no | | | | |
| Pd1 | P1 | C391 | C441 | 132.5(6) | . | . |
| . | . | no | | | | |
| C381 | P1 | C391 | C441 | -108.7(7) | . | . |
| . | . | no | | | | |
| C381 | P1 | C451 | C501 | -125.5(7) | . | . |
| . | . | no | | | | |
| C391 | P1 | C451 | C461 | -56.4(7) | . | . |
| . | . | no | | | | |
| Pd1 | P1 | C451 | C501 | -8.1(7) | . | . |

```
.       .   no
 C131    P2      C11     C21       -120.0(7)     .       .
.       .   no
 C131    P2      C71     C81       -128.2(7)     .       .
.       .   no
 Pd1     P2      C11     C61        -59.5(7)     .       .
.       .   no
 C71     P2      C11     C21        -12.2(8)     .       .
.       .   no
 Pd1     P2      C11     C21        120.1(6)     .       .
.       .   no
 C71     P2      C131    C141       -86.3(6)     .       .
.       .   no
 Pd1     P2      C71     C121       168.5(6)     .       .
.       .   no
 C11     P2      C71     C121       -57.0(8)     .       .
.       .   no
 C131    P2      C71     C121        50.1(7)     .       .
.       .   no
 C71     P2      C11     C61        168.2(6)     .       .
.       .   no
 C131    P2      C11     C61         60.4(7)     .       .
.       .   no
 C11     P2      C131    C181      -160.7(6)     .       .
.       .   no
 Pd1     P2      C131    C141       150.9(5)     .       .
.       .   no
 Pd1     P2      C131    C181       -33.7(6)     .       .
.       .   no
 Pd1     P2      C71     C81         -9.9(8)     .       .
.       .   no
 C71     P2      C131    C181        89.0(6)     .       .
.       .   no
 C11     P2      C131    C141        24.0(6)     .       .
.       .   no
 C11     P2      C71     C81        124.7(7)     .       .
.       .   no
 C191    N1      C201    C251       -96.8(9)     .       .
.       .   no
 Pd1     N1      C201    C211      -104.4(7)     .       .
.       .   no
 Pd1     N1      C201    C251        81.6(8)     .       .
.       .   no
 C191    N1      C201    C211        77.3(9)     .       .
.       .   no
 Pd1     N1      C191    C181        5.1(12)     .       .
.       .   no
 C201    N1      C191    C181      -176.9(7)     .       .
.       .   no
 Pd1     N2      C311    C261        73.1(8)     .       .
.       .   no
 C321    N2      C311    C301        67.2(9)     .       .
.       .   no
 Pd1     N2      C321    C331        5.4(10)     .       .
.       .   no
 Pd1     N2      C311    C301      -110.2(7)     .       .
.       .   no
 C311    N2      C321    C331      -171.6(7)     .       .
.       .   no
 C321    N2      C311    C261      -109.6(8)     .       .
.       .   no
 C21     C11     C61     C51        -0.6(12)     .       .
.       .   no
 P2      C11     C21     C31        179.6(6)     .       .
.       .   no
 P2      C11     C61     C51        179.1(7)     .       .
.       .   no
```

| | | | | | | |
|---|---|---|---|---|---|---|
| C61 | C11 | C21 | C31 | -0.8(11) | . | . |
| . | . | no | | | | |
| C11 | C21 | C31 | C41 | 0.9(12) | . | . |
| . | . | no | | | | |
| C21 | C31 | C41 | C51 | 0.3(13) | . | . |
| . | . | no | | | | |
| C31 | C41 | C51 | C61 | -1.7(14) | . | . |
| . | . | no | | | | |
| C41 | C51 | C61 | C11 | 1.8(13) | . | . |
| . | . | no | | | | |
| P2 | C71 | C81 | C91 | 179.7(8) | . | . |
| . | . | no | | | | |
| C121 | C71 | C81 | C91 | 1.4(13) | . | . |
| . | . | no | | | | |
| P2 | C71 | C121 | C111 | -179.6(7) | . | . |
| . | . | no | | | | |
| C81 | C71 | C121 | C111 | -1.3(13) | . | . |
| . | . | no | | | | |
| C71 | C81 | C91 | C101 | -0.6(15) | . | . |
| . | . | no | | | | |
| C81 | C91 | C101 | C111 | -0.5(15) | . | . |
| . | . | no | | | | |
| C91 | C101 | C111 | C121 | 0.6(14) | . | . |
| . | . | no | | | | |
| C101 | C111 | C121 | C71 | 0.3(15) | . | . |
| . | . | no | | | | |
| P2 | C131 | C181 | C191 | 1.4(10) | . | . |
| . | . | no | | | | |
| P2 | C131 | C181 | C171 | -175.0(6) | . | . |
| . | . | no | | | | |
| C141 | C131 | C181 | C171 | 0.4(11) | . | . |
| . | . | no | | | | |
| P2 | C131 | C141 | C151 | 175.0(6) | . | . |
| . | . | no | | | | |
| C181 | C131 | C141 | C151 | -0.6(11) | . | . |
| . | . | no | | | | |
| C141 | C131 | C181 | C191 | 176.8(7) | . | . |
| . | . | no | | | | |
| C131 | C141 | C151 | C161 | 0.9(11) | . | . |
| . | . | no | | | | |
| C141 | C151 | C161 | C171 | -1.0(12) | . | . |
| . | . | no | | | | |
| C151 | C161 | C171 | C181 | 0.8(12) | . | . |
| . | . | no | | | | |
| C161 | C171 | C181 | C191 | -177.3(7) | . | . |
| . | . | no | | | | |
| C161 | C171 | C181 | C131 | -0.5(11) | . | . |
| . | . | no | | | | |
| C131 | C181 | C191 | N1 | 18.8(13) | . | . |
| . | . | no | | | | |
| C171 | C181 | C191 | N1 | -164.7(8) | . | . |
| . | . | no | | | | |
| N1 | C201 | C211 | C221 | -173.3(8) | . | . |
| . | . | no | | | | |
| N1 | C201 | C251 | C261 | -3.1(12) | . | . |
| . | . | no | | | | |
| C251 | C201 | C211 | C221 | 0.6(13) | . | . |
| . | . | no | | | | |
| N1 | C201 | C251 | C241 | 173.0(7) | . | . |
| . | . | no | | | | |
| C211 | C201 | C251 | C261 | -177.0(8) | . | . |
| . | . | no | | | | |
| C211 | C201 | C251 | C241 | -0.8(12) | . | . |
| . | . | no | | | | |
| C201 | C211 | C221 | C231 | 0.1(17) | . | . |
| . | . | no | | | | |
| C211 | C221 | C231 | C241 | -0.6(14) | . | . |

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.       .   no
 C221    C231    C241    C251        0.3(14)     .       .
.       .   no
 C231    C241    C251    C201        0.3(12)     .       .
.       .   no
 C231    C241    C251    C261       176.6(8)     .       .
.       .   no
 C201    C251    C261    C271       124.7(9)     .       .
.       .   no
 C241    C251    C261    C311       123.6(9)     .       .
.       .   no
 C201    C251    C261    C311      -60.3(11)     .       .
.       .   no
 C241    C251    C261    C271      -51.4(11)     .       .
.       .   no
 C251    C261    C311    N2          1.7(11)     .       .
.       .   no
 C271    C261    C311    N2         176.9(7)     .       .
.       .   no
 C271    C261    C311    C301        0.2(11)     .       .
.       .   no
 C311    C261    C271    C281       -1.2(11)     .       .
.       .   no
 C251    C261    C271    C281       174.0(7)     .       .
.       .   no
 C251    C261    C311    C301      -174.9(7)     .       .
.       .   no
 C261    C271    C281    C291        1.7(12)     .       .
.       .   no
 C271    C281    C291    C301       -1.2(11)     .       .
.       .   no
 C281    C291    C301    C311        0.2(10)     .       .
.       .   no
 C291    C301    C311    C261        0.2(12)     .       .
.       .   no
 C291    C301    C311    N2        -176.5(7)     .       .
.       .   no
 N2      C321    C331    C381       23.1(11)     .       .
.       .   no
 N2      C321    C331    C341      -157.9(7)     .       .
.       .   no
 C341    C331    C381    C371        0.0(10)     .       .
.       .   no
 C381    C331    C341    C351       -0.7(11)     .       .
.       .   no
 C321    C331    C341    C351      -179.8(6)     .       .
.       .   no
 C321    C331    C381    C371       179.0(7)     .       .
.       .   no
 C341    C331    C381    P1        -178.1(5)     .       .
.       .   no
 C321    C331    C381    P1          0.8(10)     .       .
.       .   no
 C331    C341    C351    C361        0.4(11)     .       .
.       .   no
 C341    C351    C361    C371        0.7(11)     .       .
.       .   no
 C351    C361    C371    C381       -1.5(12)     .       .
.       .   no
 C361    C371    C381    C331        1.1(11)     .       .
.       .   no
 C361    C371    C381    P1         179.3(5)     .       .
.       .   no
 P1      C391    C401    C411      -175.0(6)     .       .
.       .   no
 C401    C391    C441    C431       -0.8(11)     .       .
.       .   no
```

| | | | | | | |
|---|---|---|---|---|---|---|
| C441 | C391 | C401 | C411 | 1.0(12) | . | . |
| . | . | no | | | | |
| P1 | C391 | C441 | C431 | 174.9(6) | . | . |
| . | . | no | | | | |
| C391 | C401 | C411 | C421 | -0.9(12) | . | . |
| . | . | no | | | | |
| C401 | C411 | C421 | C431 | 0.7(13) | . | . |
| . | . | no | | | | |
| C411 | C421 | C431 | C441 | -0.4(13) | . | . |
| . | . | no | | | | |
| C421 | C431 | C441 | C391 | 0.5(12) | . | . |
| . | . | no | | | | |
| P1 | C451 | C461 | C471 | 178.1(7) | . | . |
| . | . | no | | | | |
| C501 | C451 | C461 | C471 | -3.0(12) | . | . |
| . | . | no | | | | |
| P1 | C451 | C501 | C491 | -177.9(7) | . | . |
| . | . | no | | | | |
| C461 | C451 | C501 | C491 | 3.2(12) | . | . |
| . | . | no | | | | |
| C451 | C461 | C471 | C481 | 1.3(13) | . | . |
| . | . | no | | | | |
| C461 | C471 | C481 | C491 | 0.4(14) | . | . |
| . | . | no | | | | |
| C471 | C481 | C491 | C501 | -0.2(15) | . | . |
| . | . | no | | | | |
| C481 | C491 | C501 | C451 | -1.6(13) | . | . |
| . | . | no | | | | |
| P4 | Pd2 | P3 | C382 | -147.0(2) | . | . |
| . | . | no | | | | |
| P4 | Pd2 | P3 | C392 | -30.5(3) | . | . |
| . | . | no | | | | |
| P4 | Pd2 | P3 | C452 | 99.8(3) | . | . |
| . | . | no | | | | |
| N4 | Pd2 | P3 | C382 | 48.7(3) | . | . |
| . | . | no | | | | |
| N4 | Pd2 | P3 | C392 | 165.2(3) | . | . |
| . | . | no | | | | |
| N4 | Pd2 | P3 | C452 | -64.6(3) | . | . |
| . | . | no | | | | |
| P3 | Pd2 | P4 | C12 | -24.1(3) | . | . |
| . | . | no | | | | |
| P3 | Pd2 | P4 | C72 | 103.2(3) | . | . |
| . | . | no | | | | |
| P3 | Pd2 | P4 | C132 | -141.3(3) | . | . |
| . | . | no | | | | |
| N3 | Pd2 | P4 | C12 | 154.9(3) | . | . |
| . | . | no | | | | |
| N3 | Pd2 | P4 | C72 | -77.7(3) | . | . |
| . | . | no | | | | |
| N3 | Pd2 | P4 | C132 | 37.7(3) | . | . |
| . | . | no | | | | |
| P4 | Pd2 | N3 | C192 | -28.1(7) | . | . |
| . | . | no | | | | |
| P4 | Pd2 | N3 | C202 | 148.5(4) | . | . |
| . | . | no | | | | |
| N4 | Pd2 | N3 | C192 | 136.4(7) | . | . |
| . | . | no | | | | |
| N4 | Pd2 | N3 | C202 | -47.0(5) | . | . |
| . | . | no | | | | |
| P3 | Pd2 | N4 | C312 | 137.6(5) | . | . |
| . | . | no | | | | |
| P3 | Pd2 | N4 | C322 | -37.6(7) | . | . |
| . | . | no | | | | |
| N3 | Pd2 | N4 | C312 | -42.9(5) | . | . |
| . | . | no | | | | |
| N3 | Pd2 | N4 | C322 | 142.0(7) | . | . |

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.       .   no
 C452    P3      C392    C442       -0.9(8)     .       .
.       .   no
 C392    P3      C382    C372       12.6(7)     .       .
.       .   no
 C452    P3      C382    C372      -99.9(6)     .       .
.       .   no
 Pd2     P3      C392    C402      -51.0(7)     .       .
.       .   no
 Pd2     P3      C382    C332      -46.6(6)     .       .
.       .   no
 C392    P3      C382    C332     -174.1(6)     .       .
.       .   no
 C452    P3      C382    C332       73.4(6)     .       .
.       .   no
 Pd2     P3      C382    C372      140.1(5)     .       .
.       .   no
 C392    P3      C452    C502      118.8(7)     .       .
.       .   no
 C452    P3      C392    C402      176.7(6)     .       .
.       .   no
 Pd2     P3      C452    C462      161.7(6)     .       .
.       .   no
 C382    P3      C392    C402       68.4(7)     .       .
.       .   no
 C382    P3      C452    C462       45.4(7)     .       .
.       .   no
 Pd2     P3      C392    C442      131.4(6)     .       .
.       .   no
 C382    P3      C392    C442     -109.2(7)     .       .
.       .   no
 C382    P3      C452    C502     -133.3(7)     .       .
.       .   no
 C392    P3      C452    C462      -62.4(7)     .       .
.       .   no
 Pd2     P3      C452    C502      -17.0(7)     .       .
.       .   no
 C132    P4      C12     C22      -116.5(7)     .       .
.       .   no
 C132    P4      C72     C82      -136.8(7)     .       .
.       .   no
 Pd2     P4      C12     C62       -58.2(7)     .       .
.       .   no
 C72     P4      C12     C22        -8.8(8)     .       .
.       .   no
 Pd2     P4      C12     C22       123.5(6)     .       .
.       .   no
 C72     P4      C132    C142      -86.9(7)     .       .
.       .   no
 Pd2     P4      C72     C122      162.7(6)     .       .
.       .   no
 C12     P4      C72     C122      -63.9(7)     .       .
.       .   no
 C132    P4      C72     C122       44.0(7)     .       .
.       .   no
 C72     P4      C12     C62       169.5(6)     .       .
.       .   no
 C132    P4      C12     C62        61.8(7)     .       .
.       .   no
 C12     P4      C132    C182     -163.2(7)     .       .
.       .   no
 Pd2     P4      C132    C142      149.2(6)     .       .
.       .   no
 Pd2     P4      C132    C182      -36.8(7)     .       .
.       .   no
 Pd2     P4      C72     C82       -18.2(8)     .       .
.       .   no
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| | | | | | | |
|---|---|---|---|---|---|---|
| C72 | P4 | C132 | C182 | 87.1(7) | . | . |
| . | . | no | | | | |
| C12 | P4 | C132 | C142 | 22.8(7) | . | . |
| . | . | no | | | | |
| C12 | P4 | C72 | C82 | 115.2(8) | . | . |
| . | . | no | | | | |
| C192 | N3 | C202 | C252 | -103.1(8) | . | . |
| . | . | no | | | | |
| Pd2 | N3 | C202 | C212 | -104.5(7) | . | . |
| . | . | no | | | | |
| Pd2 | N3 | C202 | C252 | 79.7(8) | . | . |
| . | . | no | | | | |
| C192 | N3 | C202 | C212 | 72.7(10) | . | . |
| . | . | no | | | | |
| Pd2 | N3 | C192 | C182 | 0.4(13) | . | . |
| . | . | no | | | | |
| C202 | N3 | C192 | C182 | -176.2(7) | . | . |
| . | . | no | | | | |
| Pd2 | N4 | C312 | C262 | 74.4(8) | . | . |
| . | . | no | | | | |
| C322 | N4 | C312 | C302 | 65.5(9) | . | . |
| . | . | no | | | | |
| Pd2 | N4 | C322 | C332 | 3.9(12) | . | . |
| . | . | no | | | | |
| Pd2 | N4 | C312 | C302 | -110.3(7) | . | . |
| . | . | no | | | | |
| C312 | N4 | C322 | C332 | -171.2(7) | . | . |
| . | . | no | | | | |
| C322 | N4 | C312 | C262 | -109.7(8) | . | . |
| . | . | no | | | | |
| C22 | C12 | C62 | C52 | -1.6(12) | . | . |
| . | . | no | | | | |
| P4 | C12 | C22 | C32 | -179.5(6) | . | . |
| . | . | no | | | | |
| P4 | C12 | C62 | C52 | -180.0(7) | . | . |
| . | . | no | | | | |
| C62 | C12 | C22 | C32 | 2.3(12) | . | . |
| . | . | no | | | | |
| C12 | C22 | C32 | C42 | -1.5(12) | . | . |
| . | . | no | | | | |
| C22 | C32 | C42 | C52 | 0.0(13) | . | . |
| . | . | no | | | | |
| C32 | C42 | C52 | C62 | 0.6(14) | . | . |
| . | . | no | | | | |
| C42 | C52 | C62 | C12 | 0.2(15) | . | . |
| . | . | no | | | | |
| P4 | C72 | C82 | C92 | -177.4(8) | . | . |
| . | . | no | | | | |
| C122 | C72 | C82 | C92 | 1.8(14) | . | . |
| . | . | no | | | | |
| P4 | C72 | C122 | C112 | 179.1(7) | . | . |
| . | . | no | | | | |
| C82 | C72 | C122 | C112 | -0.1(13) | . | . |
| . | . | no | | | | |
| C72 | C82 | C92 | C102 | -2.2(16) | . | . |
| . | . | no | | | | |
| C82 | C92 | C102 | C112 | 0.9(15) | . | . |
| . | . | no | | | | |
| C92 | C102 | C112 | C122 | 0.8(15) | . | . |
| . | . | no | | | | |
| C102 | C112 | C122 | C72 | -1.2(14) | . | . |
| . | . | no | | | | |
| P4 | C132 | C182 | C192 | 5.4(11) | . | . |
| . | . | no | | | | |
| P4 | C132 | C182 | C172 | -173.5(6) | . | . |
| . | . | no | | | | |
| C142 | C132 | C182 | C172 | 0.5(11) | . | . |

```
.       .   no
 P4     C132    C142    C152       174.9(6)     .       .
.       .   no
 C182   C132    C142    C152        0.7(12)     .       .
.       .   no
 C142   C132    C182    C192       179.4(7)     .       .
.       .   no
 C132   C142    C152    C162       -0.7(12)     .       .
.       .   no
 C142   C152    C162    C172       -0.5(12)     .       .
.       .   no
 C152   C162    C172    C182        1.7(12)     .       .
.       .   no
 C162   C172    C182    C192       179.3(7)     .       .
.       .   no
 C162   C172    C182    C132       -1.7(12)     .       .
.       .   no
 C132   C182    C192    N3         18.8(13)     .       .
.       .   no
 C172   C182    C192    N3        -162.2(8)     .       .
.       .   no
 N3     C202    C212    C222      -173.8(8)     .       .
.       .   no
 N3     C202    C252    C262       -2.1(12)     .       .
.       .   no
 C252   C202    C212    C222        1.9(13)     .       .
.       .   no
 N3     C202    C252    C242       172.6(7)     .       .
.       .   no
 C212   C202    C252    C262      -177.8(8)     .       .
.       .   no
 C212   C202    C252    C242       -3.1(12)     .       .
.       .   no
 C202   C212    C222    C232       -0.4(14)     .       .
.       .   no
 C212   C222    C232    C242        0.2(14)     .       .
.       .   no
 C222   C232    C242    C252       -1.4(13)     .       .
.       .   no
 C232   C242    C252    C202        2.8(12)     .       .
.       .   no
 C232   C242    C252    C262       177.7(8)     .       .
.       .   no
 C202   C252    C262    C272       123.1(9)     .       .
.       .   no
 C242   C252    C262    C312       123.9(9)     .       .
.       .   no
 C202   C252    C262    C312      -61.5(11)     .       .
.       .   no
 C242   C252    C262    C272      -51.5(11)     .       .
.       .   no
 C252   C262    C312    N4          0.7(11)     .       .
.       .   no
 C272   C262    C312    N4         176.3(7)     .       .
.       .   no
 C272   C262    C312    C302        1.3(12)     .       .
.       .   no
 C312   C262    C272    C282        0.0(13)     .       .
.       .   no
 C252   C262    C272    C282       175.8(8)     .       .
.       .   no
 C252   C262    C312    C302      -174.3(7)     .       .
.       .   no
 C262   C272    C282    C292       -1.5(14)     .       .
.       .   no
 C272   C282    C292    C302        1.6(14)     .       .
.       .   no
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 C282    C292    C302    C312       -0.3(13)     .       .
.       .   no
 C292    C302    C312    C262       -1.2(12)     .       .
.       .   no
 C292    C302    C312    N4        -176.3(7)     .       .
.       .   no
 N4      C322    C332    C382       21.6(13)     .       .
.       .   no
 N4      C322    C332    C342      -159.5(8)     .       .
.       .   no
 C342    C332    C382    C372        0.5(11)     .       .
.       .   no
 C382    C332    C342    C352       -1.2(11)     .       .
.       .   no
 C322    C332    C342    C352       179.9(9)     .       .
.       .   no
 C322    C332    C382    C372       179.3(7)     .       .
.       .   no
 C342    C332    C382    P3        -173.0(6)     .       .
.       .   no
 C322    C332    C382    P3          5.8(10)     .       .
.       .   no
 C332    C342    C352    C362        0.5(12)     .       .
.       .   no
 C342    C352    C362    C372        0.9(12)     .       .
.       .   no
 C352    C362    C372    C382       -1.6(12)     .       .
.       .   no
 C362    C372    C382    C332        0.9(11)     .       .
.       .   no
 C362    C372    C382    P3         174.3(6)     .       .
.       .   no
 P3      C392    C402    C412      -177.2(6)     .       .
.       .   no
 C402    C392    C442    C432       -1.5(11)     .       .
.       .   no
 C442    C392    C402    C412        0.5(12)     .       .
.       .   no
 P3      C392    C442    C432       176.0(6)     .       .
.       .   no
 C392    C402    C412    C422        1.0(12)     .       .
.       .   no
 C402    C412    C422    C432       -1.5(13)     .       .
.       .   no
 C412    C422    C432    C442        0.5(13)     .       .
.       .   no
 C422    C432    C442    C392        1.1(12)     .       .
.       .   no
 P3      C452    C462    C472      -179.3(7)     .       .
.       .   no
 C502    C452    C462    C472       -0.6(12)     .       .
.       .   no
 P3      C452    C502    C492       179.3(7)     .       .
.       .   no
 C462    C452    C502    C492        0.5(11)     .       .
.       .   no
 C452    C462    C472    C482        0.5(13)     .       .
.       .   no
 C462    C472    C482    C492       -0.3(15)     .       .
.       .   no
 C472    C482    C492    C502        0.3(14)     .       .
.       .   no
 C482    C492    C502    C452       -0.4(14)     .       .
.       .   no

loop_
_geom_contact_atom_site_label_1
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_geom_contact_distance
_geom_contact_site_symmetry_1
_geom_contact_site_symmetry_2
_geom_contact_publ_flag
 Pd2     Cl2      2.9361(19)                    .       .
          no
 Pd2     Cl8        4.114(3)                    .       .
          no
 Cl1     C211       3.457(9)                    .       .
          no
 Cl1     C331       3.322(8)                    .       .
          no
 Cl1     C81        3.371(8)                    .       .
          no
 Cl1     C492      3.565(10)                    .     1_556
          no
 Cl1     C342       3.417(8)                    .     2_556
          no
 Cl1     C401       3.590(8)                    .       .
          no
 Cl1     C352       3.411(8)                    .     2_556
          no
 Cl2     C212      3.506(10)                    .       .
          no
 Cl2     C332       3.435(8)                    .       .
          no
 Cl2     Pd2      2.9361(19)                    .       .
          no
 Cl2     C341       3.521(8)                    .     2_556
          no
 Cl2     C351       3.466(8)                    .     2_556
          no
 Cl2     C382       3.272(7)                    .       .
          no
 Cl2     C82        3.369(8)                    .       .
          no
 Cl2     C202       3.533(8)                    .       .
          no
 Cl2     P3         3.604(3)                    .       .
          no
 Cl3     C112       3.646(9)                    .       .
          no
 Cl3     C122       3.647(8)                    .       .
          no
 Cl3     C421      3.538(10)                    .     2_566
          no
 Cl3     C6        3.450(12)                    .       .
          no
 Cl3     C191       3.405(9)                    .     2_666
          no
 Cl3     C7        3.591(12)                    .       .
          no
 Cl4     C422      3.599(10)                    .       .
          no
 Cl4     C111      3.564(10)                    .     2_666
          no
 Cl4     C5        3.507(18)                    .       .
          no
 Cl4     C192       3.368(9)                    .       .
          no
 Cl4     C3        3.472(12)                    .       .
          no
 Cl4     C2        3.613(11)                    .       .
          no
 Cl5     C301       3.444(8)                    .       .
          no
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| | | | | |
|---|---|---|---|---|
| Cl5 | C181 | 3.567(8) | . | . |
| | no | | | |
| Cl5 | C281 | 3.573(8) | . | . |
| | no | | | |
| Cl5 | C291 | 3.378(8) | . | . |
| | no | | | |
| Cl6 | C212 | 3.468(8) | . | . |
| | no | | | |
| Cl6 | C161 | 3.339(8) | . | . |
| | no | | | |
| Cl7 | C101 | 3.610(10) | . | 2_666 |
| | no | | | |
| Cl7 | C211 | 3.649(9) | . | . |
| | no | | | |
| Cl7 | C172 | 3.580(8) | . | . |
| | no | | | |
| Cl7 | C111 | 3.620(9) | . | 2_666 |
| | no | | | |
| Cl7 | C152 | 3.620(9) | . | . |
| | no | | | |
| Cl7 | C162 | 3.569(9) | . | . |
| | no | | | |
| Cl7 | Cl22 | 3.53(3) | . | . |
| | no | | | |
| Cl8 | C132 | 3.639(8) | . | . |
| | no | | | |
| Cl8 | Pd2 | 4.114(3) | . | . |
| | no | | | |
| Cl8 | C302 | 3.551(8) | . | . |
| | no | | | |
| Cl8 | C182 | 3.436(8) | . | . |
| | no | | | |
| Cl9 | Cl11 | 3.661(4) | . | . |
| | no | | | |
| Cl10 | Cl11 | 3.679(5) | . | . |
| | no | | | |
| Cl10 | C481 | 3.525(11) | . | . |
| | no | | | |
| Cl10 | C471 | 3.554(10) | . | . |
| | no | | | |
| Cl10 | C412 | 3.548(10) | . | . |
| | no | | | |
| Cl11 | C112 | 3.630(9) | . | 2_666 |
| | no | | | |
| Cl11 | Cl10 | 3.679(5) | . | . |
| | no | | | |
| Cl11 | C3 | 3.513(12) | . | . |
| | no | | | |
| Cl11 | Cl9 | 3.661(4) | . | . |
| | no | | | |
| Cl12 | Cl18 | 3.032(13) | . | . |
| | no | | | |
| Cl13 | Cl20 | 3.629(18) | . | . |
| | no | | | |
| Cl14 | Cl17 | 3.54(3) | . | . |
| | no | | | |
| Cl16 | C7 | 3.614(15) | . | . |
| | no | | | |
| Cl16 | C482 | 3.614(15) | . | . |
| | no | | | |
| Cl16 | C472 | 3.577(13) | . | . |
| | no | | | |
| Cl17 | Cl14 | 3.54(3) | . | 2_656 |
| | no | | | |
| Cl18 | Cl12 | 3.032(13) | . | . |
| | no | | | |
| Cl20 | Cl13 | 3.629(18) | . | . |

| | | | | |
|---|---|---|---|---|
| | no | | | |
| Cl21 | C472 | 3.52(4) | . | . |
| | no | | | |
| Cl22 | Cl7 | 3.53(3) | . | 2_665 |
| | no | | | |
| P3 | Cl2 | 3.604(3) | . | . |
| | no | | | |
| C2 | C172 | 3.394(13) | . | . |
| | no | | | |
| C2 | C182 | 3.585(13) | . | . |
| | no | | | |
| C2 | Cl4 | 3.613(11) | . | . |
| | no | | | |
| C3 | Cl4 | 3.472(12) | . | . |
| | no | | | |
| C3 | Cl11 | 3.513(12) | . | . |
| | no | | | |
| C5 | Cl4 | 3.507(18) | . | . |
| | no | | | |
| C6 | Cl3 | 3.450(12) | . | 2_666 |
| | no | | | |
| C7 | Cl3 | 3.591(12) | . | . |
| | no | | | |
| C7 | Cl16 | 3.614(15) | . | . |
| | no | | | |
| C11 | C441 | 3.469(11) | . | . |
| | no | | | |
| C11 | C391 | 3.244(11) | . | . |
| | no | | | |
| C12 | C442 | 3.491(11) | . | . |
| | no | | | |
| C12 | C392 | 3.203(11) | . | . |
| | no | | | |
| C21 | C431 | 3.501(11) | . | . |
| | no | | | |
| C21 | C121 | 3.272(11) | . | . |
| | no | | | |
| C21 | C391 | 3.354(11) | . | . |
| | no | | | |
| C21 | C441 | 3.272(11) | . | . |
| | no | | | |
| C22 | C442 | 3.430(11) | . | . |
| | no | | | |
| C22 | C392 | 3.386(11) | . | . |
| | no | | | |
| C22 | C432 | 3.587(12) | . | . |
| | no | | | |
| C22 | C122 | 3.293(11) | . | . |
| | no | | | |
| C22 | C402 | 3.481(11) | . | . |
| | no | | | |
| C31 | C441 | 3.408(11) | . | . |
| | no | | | |
| C31 | C431 | 3.367(11) | . | . |
| | no | | | |
| C32 | C432 | 3.305(12) | . | . |
| | no | | | |
| C32 | C442 | 3.457(11) | . | . |
| | no | | | |
| C42 | C442 | 3.570(12) | . | . |
| | no | | | |
| C61 | C501 | 3.287(11) | . | . |
| | no | | | |
| C61 | C141 | 3.242(12) | . | . |
| | no | | | |
| C61 | C451 | 3.564(11) | . | . |
| | no | | | |

| | | | | |
|---|---|---|---|---|
| C62 | C142 | 3.272(13) | . | . |
| | no | | | |
| C62 | C502 | 3.394(11) | . | . |
| | no | | | |
| C81 | Cl1 | 3.371(8) | . | . |
| | no | | | |
| C81 | C401 | 3.505(12) | . | . |
| | no | | | |
| C82 | C402 | 3.531(12) | . | . |
| | no | | | |
| C82 | Cl2 | 3.369(8) | . | . |
| | no | | | |
| C101 | Cl7 | 3.610(10) | . | 2_666 |
| | no | | | |
| C111 | Cl4 | 3.564(10) | . | 2_666 |
| | no | | | |
| C111 | Cl7 | 3.620(9) | . | 2_666 |
| | no | | | |
| C112 | Cl3 | 3.646(9) | . | . |
| | no | | | |
| C112 | Cl11 | 3.630(9) | . | 2_666 |
| | no | | | |
| C121 | C141 | 3.467(11) | . | . |
| | no | | | |
| C121 | C172 | 3.575(12) | . | 2_666 |
| | no | | | |
| C121 | C21 | 3.272(11) | . | . |
| | no | | | |
| C122 | Cl3 | 3.647(8) | . | . |
| | no | | | |
| C122 | C142 | 3.393(11) | . | . |
| | no | | | |
| C122 | C22 | 3.293(11) | . | . |
| | no | | | |
| C122 | C171 | 3.431(12) | . | 2_666 |
| | no | | | |
| C132 | Cl8 | 3.639(8) | . | . |
| | no | | | |
| C141 | C61 | 3.242(12) | . | . |
| | no | | | |
| C141 | C121 | 3.467(11) | . | . |
| | no | | | |
| C142 | C62 | 3.272(13) | . | . |
| | no | | | |
| C142 | C122 | 3.393(11) | . | . |
| | no | | | |
| C152 | Cl7 | 3.620(9) | . | 2_665 |
| | no | | | |
| C161 | Cl6 | 3.339(8) | . | . |
| | no | | | |
| C161 | C182 | 3.466(11) | . | 2_666 |
| | no | | | |
| C161 | C192 | 3.572(11) | . | 2_666 |
| | no | | | |
| C162 | C181 | 3.528(11) | . | 2_666 |
| | no | | | |
| C162 | Cl7 | 3.569(9) | . | . |
| | no | | | |
| C171 | C122 | 3.431(12) | . | 2_666 |
| | no | | | |
| C171 | C172 | 3.490(11) | . | 2_666 |
| | no | | | |
| C172 | Cl7 | 3.580(8) | . | . |
| | no | | | |
| C172 | C171 | 3.490(11) | . | 2_666 |
| | no | | | |
| C172 | C2 | 3.394(13) | . | . |

| | | | | |
|---|---|---|---|---|
| | no | | | |
| C172 | C121 | 3.575(12) | . | 2_666 |
| | no | | | |
| C181 | C162 | 3.528(11) | . | 2_666 |
| | no | | | |
| C181 | Cl5 | 3.567(8) | . | . |
| | no | | | |
| C182 | Cl8 | 3.436(8) | . | . |
| | no | | | |
| C182 | C2 | 3.585(13) | . | . |
| | no | | | |
| C182 | C161 | 3.466(11) | . | 2_666 |
| | no | | | |
| C191 | C261 | 3.521(11) | . | . |
| | no | | | |
| C191 | Cl3 | 3.405(9) | . | 2_666 |
| | no | | | |
| C192 | C262 | 3.586(11) | . | . |
| | no | | | |
| C192 | Cl4 | 3.368(9) | . | . |
| | no | | | |
| C192 | C161 | 3.572(11) | . | 2_666 |
| | no | | | |
| C202 | Cl2 | 3.533(8) | . | . |
| | no | | | |
| C211 | Cl1 | 3.457(9) | . | . |
| | no | | | |
| C211 | Cl7 | 3.649(9) | . | 1_556 |
| | no | | | |
| C212 | Cl6 | 3.468(8) | . | . |
| | no | | | |
| C212 | Cl2 | 3.506(10) | . | . |
| | no | | | |
| C231 | C362 | 3.575(13) | . | 2_556 |
| | no | | | |
| C232 | C361 | 3.584(12) | . | 2_556 |
| | no | | | |
| C241 | C362 | 3.553(11) | . | 2_556 |
| | no | | | |
| C242 | C361 | 3.559(11) | . | 2_556 |
| | no | | | |
| C261 | C191 | 3.521(11) | . | . |
| | no | | | |
| C262 | C192 | 3.586(11) | . | . |
| | no | | | |
| C281 | Cl5 | 3.573(8) | . | . |
| | no | | | |
| C291 | Cl5 | 3.378(8) | . | . |
| | no | | | |
| C291 | C461 | 3.416(11) | . | 2_556 |
| | no | | | |
| C291 | C341 | 3.532(10) | . | 2_556 |
| | no | | | |
| C301 | Cl5 | 3.444(8) | . | . |
| | no | | | |
| C302 | Cl8 | 3.551(8) | . | . |
| | no | | | |
| C302 | C502 | 3.553(13) | . | . |
| | no | | | |
| C322 | C452 | 3.552(11) | . | . |
| | no | | | |
| C331 | Cl1 | 3.322(8) | . | . |
| | no | | | |
| C332 | Cl2 | 3.435(8) | . | . |
| | no | | | |
| C341 | C291 | 3.532(10) | . | 2_556 |
| | no | | | |

| | | | | |
|---|---|---|---|---|
| C341 | C342 | 3.231(10) | . | 2_556 |
| | no | | | |
| C341 | C352 | 3.576(11) | . | 2_556 |
| | no | | | |
| C341 | Cl2 | 3.521(8) | . | 2_556 |
| | no | | | |
| C342 | Cl1 | 3.417(8) | . | 2_556 |
| | no | | | |
| C342 | C351 | 3.588(11) | . | 2_556 |
| | no | | | |
| C342 | C341 | 3.231(10) | . | 2_556 |
| | no | | | |
| C351 | C342 | 3.588(11) | . | 2_556 |
| | no | | | |
| C351 | Cl2 | 3.466(8) | . | 2_556 |
| | no | | | |
| C352 | C341 | 3.576(11) | . | 2_556 |
| | no | | | |
| C352 | Cl1 | 3.411(8) | . | 2_556 |
| | no | | | |
| C361 | C242 | 3.559(11) | . | 2_556 |
| | no | | | |
| C361 | C232 | 3.584(12) | . | 2_556 |
| | no | | | |
| C362 | C241 | 3.553(11) | . | 2_556 |
| | no | | | |
| C362 | C231 | 3.575(13) | . | 2_556 |
| | no | | | |
| C371 | C401 | 3.259(11) | . | . |
| | no | | | |
| C372 | C402 | 3.252(11) | . | . |
| | no | | | |
| C382 | Cl2 | 3.272(7) | . | . |
| | no | | | |
| C391 | C21 | 3.354(11) | . | . |
| | no | | | |
| C391 | C11 | 3.244(11) | . | . |
| | no | | | |
| C392 | C22 | 3.386(11) | . | . |
| | no | | | |
| C392 | C12 | 3.203(11) | . | . |
| | no | | | |
| C401 | C81 | 3.505(12) | . | . |
| | no | | | |
| C401 | Cl1 | 3.590(8) | . | . |
| | no | | | |
| C401 | C371 | 3.259(11) | . | . |
| | no | | | |
| C402 | C372 | 3.252(11) | . | . |
| | no | | | |
| C402 | C82 | 3.531(12) | . | . |
| | no | | | |
| C402 | C22 | 3.481(11) | . | . |
| | no | | | |
| C412 | Cl10 | 3.548(10) | . | 1_455 |
| | no | | | |
| C421 | Cl3 | 3.538(10) | . | 2_566 |
| | no | | | |
| C422 | Cl4 | 3.599(10) | . | 1_455 |
| | no | | | |
| C431 | C31 | 3.367(11) | . | . |
| | no | | | |
| C431 | C21 | 3.501(11) | . | . |
| | no | | | |
| C432 | C22 | 3.587(12) | . | . |
| | no | | | |
| C432 | C32 | 3.305(12) | . | . |

| | | | | |
|---|---|---|---|---|
| | no | | | |
| C441 | C11 | 3.469(11) | . | . |
| | no | | | |
| C441 | C21 | 3.272(11) | . | . |
| | no | | | |
| C441 | C31 | 3.408(11) | . | . |
| | no | | | |
| C441 | C461 | 3.275(11) | . | . |
| | no | | | |
| C442 | C42 | 3.570(12) | . | . |
| | no | | | |
| C442 | C32 | 3.457(11) | . | . |
| | no | | | |
| C442 | C22 | 3.430(11) | . | . |
| | no | | | |
| C442 | C12 | 3.491(11) | . | . |
| | no | | | |
| C442 | C462 | 3.332(11) | . | . |
| | no | | | |
| C451 | C61 | 3.564(11) | . | . |
| | no | | | |
| C452 | C322 | 3.552(11) | . | . |
| | no | | | |
| C461 | C291 | 3.416(11) | . | 2_556 |
| | no | | | |
| C461 | C441 | 3.275(11) | . | . |
| | no | | | |
| C462 | C442 | 3.332(11) | . | . |
| | no | | | |
| C471 | Cl10 | 3.554(10) | . | 1_455 |
| | no | | | |
| C472 | Cl21 | 3.52(4) | . | . |
| | no | | | |
| C472 | Cl16 | 3.577(13) | . | 1_454 |
| | no | | | |
| C481 | Cl10 | 3.525(11) | . | 1_455 |
| | no | | | |
| C482 | Cl16 | 3.614(15) | . | 1_454 |
| | no | | | |
| C492 | Cl1 | 3.565(10) | . | . |
| | no | | | |
| C501 | C61 | 3.287(11) | . | . |
| | no | | | |
| C502 | C62 | 3.394(11) | . | . |
| | no | | | |
| C502 | C302 | 3.553(13) | . | . |
| | no | | | |
| Pd1 | H81 | 3.02(3) | . | . |
| | no | | | |
| Pd1 | H401 | 3.38(6) | . | . |
| | no | | | |
| Pd1 | H61 | 3.68(4) | . | . |
| | no | | | |
| Pd1 | H501 | 2.96(4) | . | . |
| | no | | | |
| Pd2 | H62 | 3.66(5) | . | . |
| | no | | | |
| Pd2 | H82 | 3.17(4) | . | . |
| | no | | | |
| Pd2 | H502 | 2.99(4) | . | . |
| | no | | | |
| Pd2 | H402 | 3.55(6) | . | . |
| | no | | | |
| Cl1 | H492 | 2.73(6) | . | 1_556 |
| | no | | | |
| Cl1 | H352 | 2.82(7) | . | 2_556 |
| | no | | | |

| | | | | |
|---|---|---|---|---|
| Cl1 | H81 | 2.39(9) | . | . |
| | no | | | |
| Cl1 | H401 | 2.68(5) | . | . |
| | no | | | |
| Cl1 | H342 | 2.87(5) | . | 2_556 |
| | no | | | |
| Cl2 | H82 | 2.42(9) | . | . |
| | no | | | |
| Cl2 | H201 | 2.8412 | . | . |
| | no | | | |
| Cl2 | H341 | 2.90(5) | . | 2_556 |
| | no | | | |
| Cl2 | H491 | 3.01(5) | . | . |
| | no | | | |
| Cl2 | H351 | 2.81(7) | . | 2_556 |
| | no | | | |
| Cl2 | H402 | 3.06(5) | . | . |
| | no | | | |
| Cl3 | H340 | 2.6774 | . | . |
| | no | | | |
| Cl3 | H310 | 3.1066 | . | . |
| | no | | | |
| Cl3 | H122 | 3.04(4) | . | . |
| | no | | | |
| Cl3 | H620 | 2.7044 | . | . |
| | no | | | |
| Cl3 | H360 | 2.8782 | . | . |
| | no | | | |
| Cl3 | H112 | 2.97(7) | . | . |
| | no | | | |
| Cl3 | H630 | 2.7381 | . | . |
| | no | | | |
| Cl3 | H14 | 2.7903 | . | 2_666 |
| | no | | | |
| Cl3 | H421 | 3.04(5) | . | 2_566 |
| | no | | | |
| Cl3 | H171 | 3.13(4) | . | 2_666 |
| | no | | | |
| Cl3 | H191 | 2.60(7) | . | 2_666 |
| | no | | | |
| Cl4 | H12 | 2.7395 | . | . |
| | no | | | |
| Cl4 | H422 | 3.07(5) | . | . |
| | no | | | |
| Cl4 | H203 | 2.5534 | . | . |
| | no | | | |
| Cl4 | H111 | 2.89(7) | . | 2_666 |
| | no | | | |
| Cl4 | H205 | 2.5645 | . | . |
| | no | | | |
| Cl4 | H172 | 2.83(4) | . | . |
| | no | | | |
| Cl4 | H192 | 2.62(7) | . | . |
| | no | | | |
| Cl6 | H212 | 2.73(4) | . | . |
| | no | | | |
| Cl6 | H222 | 3.13(5) | . | . |
| | no | | | |
| Cl7 | H152 | 2.93(5) | . | . |
| | no | | | |
| Cl7 | H211 | 2.98(4) | . | . |
| | no | | | |
| Cl8 | H502 | 2.92(9) | . | . |
| | no | | | |
| Cl9 | H141 | 2.97(4) | . | 2_666 |
| | no | | | |
| Cl11 | H13 | 3.0186 | . | . |

| | | | | |
|---|---|---|---|---|
| | no | | | |
| Cl11 | H431 | 2.97(4) | . | . |
| | no | | | |
| Cl11 | H102 | 3.12(6) | . | 2_666 |
| | no | | | |
| Cl11 | H112 | 2.94(5) | . | 2_666 |
| | no | | | |
| Cl12 | H281 | 2.92(6) | . | . |
| | no | | | |
| Cl13 | H462 | 3.14(6) | . | . |
| | no | | | |
| Cl14 | H231 | 3.14(5) | . | . |
| | no | | | |
| Cl15 | H232 | 2.99(5) | . | . |
| | no | | | |
| Cl15 | H241 | 3.03(3) | . | . |
| | no | | | |
| Cl16 | H361 | 3.08(5) | . | . |
| | no | | | |
| Cl16 | H472 | 3.11(6) | . | . |
| | no | | | |
| Cl17 | H242 | 3.00(7) | . | . |
| | no | | | |
| Cl18 | H271 | 3.13(9) | . | . |
| | no | | | |
| Cl19 | H421 | 3.04(4) | . | 2_566 |
| | no | | | |
| Cl19 | H142 | 2.91(5) | . | . |
| | no | | | |
| Cl19 | H42 | 2.90(4) | . | . |
| | no | | | |
| Cl22 | H111 | 3.11(5) | . | . |
| | no | | | |
| C1 | H212 | 3.06(4) | . | . |
| | no | | | |
| C2 | H221 | 3.07(8) | . | . |
| | no | | | |
| C5 | H372 | 3.09(4) | . | . |
| | no | | | |
| C5 | H272 | 3.02(9) | . | . |
| | no | | | |
| C11 | H141 | 2.54(5) | . | . |
| | no | | | |
| C12 | H142 | 2.55(6) | . | . |
| | no | | | |
| C21 | H121 | 3.08(4) | . | . |
| | no | | | |
| C61 | H141 | 2.77(4) | . | . |
| | no | | | |
| C62 | H502 | 3.06(6) | . | . |
| | no | | | |
| C62 | H142 | 2.80(5) | . | . |
| | no | | | |
| C71 | H21 | 2.69(4) | . | . |
| | no | | | |
| C72 | H22 | 2.63(4) | . | . |
| | no | | | |
| C81 | H401 | 2.92(5) | . | . |
| | no | | | |
| C82 | H402 | 3.01(5) | . | . |
| | no | | | |
| C111 | H172 | 3.06(6) | . | 2_666 |
| | no | | | |
| C112 | H431 | 2.95(5) | . | 2_566 |
| | no | | | |
| C112 | H171 | 2.95(6) | . | 2_666 |
| | no | | | |

| | | | | |
|---|---|---|---|---|
| C121 | H21 | 2.71(5) | . | . |
| | no | | | |
| C121 | H172 | 2.82(6) | . | 2_666 |
| | no | | | |
| C122 | H22 | 2.72(5) | . | . |
| | no | | | |
| C122 | H171 | 2.79(6) | . | 2_666 |
| | no | | | |
| C131 | H61 | 3.04(4) | . | . |
| | no | | | |
| C131 | H121 | 2.98(5) | . | . |
| | no | | | |
| C132 | H122 | 2.83(5) | . | . |
| | no | | | |
| C141 | H121 | 2.92(5) | . | . |
| | no | | | |
| C142 | H122 | 2.74(5) | . | . |
| | no | | | |
| C172 | H12 | 2.7903 | . | . |
| | no | | | |
| C182 | H12 | 2.9970 | . | . |
| | no | | | |
| C191 | H211 | 3.04(5) | . | . |
| | no | | | |
| C192 | H212 | 2.95(5) | . | . |
| | no | | | |
| C192 | H12 | 2.9904 | . | . |
| | no | | | |
| C211 | H191 | 2.87(3) | . | . |
| | no | | | |
| C212 | H192 | 2.78(3) | . | . |
| | no | | | |
| C221 | H202 | 3.0050 | . | 1_556 |
| | no | | | |
| C222 | H13 | 2.9599 | . | . |
| | no | | | |
| C231 | H362 | 3.00(4) | . | 2_556 |
| | no | | | |
| C232 | H361 | 2.98(4) | . | 2_556 |
| | no | | | |
| C232 | H13 | 3.0397 | . | . |
| | no | | | |
| C241 | H630 | 3.0207 | . | . |
| | no | | | |
| C241 | H620 | 3.0796 | . | . |
| | no | | | |
| C241 | H271 | 2.88(5) | . | . |
| | no | | | |
| C241 | H362 | 2.87(4) | . | 2_556 |
| | no | | | |
| C241 | H352 | 3.07(6) | . | 2_556 |
| | no | | | |
| C242 | H272 | 2.87(5) | . | . |
| | no | | | |
| C242 | H361 | 2.86(4) | . | 2_556 |
| | no | | | |
| C271 | H241 | 2.87(5) | . | . |
| | no | | | |
| C272 | H242 | 2.87(5) | . | . |
| | no | | | |
| C281 | H204 | 2.9167 | . | . |
| | no | | | |
| C282 | H202 | 2.9486 | . | . |
| | no | | | |
| C301 | H321 | 2.79(5) | . | . |
| | no | | | |
| C302 | H322 | 2.76(5) | . | . |

| | | | | |
|---|---|---|---|---|
| | no | | | |
| C321 | H301 | 2.86(4) | . | . |
| | no | | | |
| C322 | H302 | 2.86(5) | . | . |
| | no | | | |
| C331 | H291 | 2.93(6) | . | 2_556 |
| | no | | | |
| C341 | H291 | 2.80(7) | . | 2_556 |
| | no | | | |
| C342 | H292 | 2.93(7) | . | 2_555 |
| | no | | | |
| C351 | H291 | 2.80(8) | . | 2_556 |
| | no | | | |
| C352 | H292 | 2.90(8) | . | 2_555 |
| | no | | | |
| C361 | H482 | 3.02(9) | . | 1_556 |
| | no | | | |
| C361 | H291 | 2.91(8) | . | 2_556 |
| | no | | | |
| C362 | H481 | 3.09(9) | . | . |
| | no | | | |
| C371 | H291 | 3.01(7) | . | 2_556 |
| | no | | | |
| C372 | H462 | 3.04(4) | . | . |
| | no | | | |
| C372 | H15 | 3.0609 | . | 1_455 |
| | no | | | |
| C381 | H291 | 3.05(6) | . | 2_556 |
| | no | | | |
| C381 | H461 | 3.04(5) | . | . |
| | no | | | |
| C382 | H462 | 2.89(5) | . | . |
| | no | | | |
| C391 | H371 | 2.55(5) | . | . |
| | no | | | |
| C392 | H372 | 2.48(5) | . | . |
| | no | | | |
| C401 | H371 | 2.78(5) | . | . |
| | no | | | |
| C402 | H372 | 2.65(5) | . | . |
| | no | | | |
| C412 | H31 | 3.09(5) | . | 2_566 |
| | no | | | |
| C432 | H15 | 3.0435 | . | 1_455 |
| | no | | | |
| C441 | H461 | 2.99(3) | . | . |
| | no | | | |
| C451 | H441 | 2.76(3) | . | . |
| | no | | | |
| C452 | H442 | 2.71(3) | . | . |
| | no | | | |
| C461 | H441 | 2.62(5) | . | . |
| | no | | | |
| C462 | H442 | 2.70(5) | . | . |
| | no | | | |
| C481 | H321 | 2.92(6) | . | 2_556 |
| | no | | | |
| C482 | H322 | 3.02(7) | . | 2_555 |
| | no | | | |
| C491 | H321 | 3.07(7) | . | 2_556 |
| | no | | | |
| C491 | H341 | 3.06(3) | . | 2_556 |
| | no | | | |
| C501 | H61 | 2.69(4) | . | . |
| | no | | | |
| C501 | H301 | 2.95(6) | . | . |
| | no | | | |

| | | | | |
|---|---|---|---|---|
| C502 | H302 | 2.95(6) | . | . |
| | no | | | |
| C502 | H62 | 2.79(5) | . | . |
| | no | | | |
| H12 | Cl4 | 2.7395 | . | . |
| | no | | | |
| H12 | H172 | 2.5930 | . | . |
| | no | | | |
| H12 | C192 | 2.9904 | . | . |
| | no | | | |
| H12 | C172 | 2.7903 | . | . |
| | no | | | |
| H12 | C182 | 2.9970 | . | . |
| | no | | | |
| H13 | Cl11 | 3.0186 | . | . |
| | no | | | |
| H13 | C232 | 3.0397 | . | . |
| | no | | | |
| H13 | C222 | 2.9599 | . | . |
| | no | | | |
| H14 | H431 | 2.5580 | . | . |
| | no | | | |
| H14 | Cl3 | 2.7903 | . | 2_666 |
| | no | | | |
| H15 | C372 | 3.0609 | . | . |
| | no | | | |
| H15 | H372 | 2.2330 | . | . |
| | no | | | |
| H15 | C432 | 3.0435 | . | . |
| | no | | | |
| H21 | H32 | 2.57(8) | . | 2_566 |
| | no | | | |
| H21 | C121 | 2.71(5) | . | . |
| | no | | | |
| H21 | C71 | 2.69(4) | . | . |
| | no | | | |
| H22 | C122 | 2.72(5) | . | . |
| | no | | | |
| H22 | C72 | 2.63(4) | . | . |
| | no | | | |
| H31 | C412 | 3.09(5) | . | 2_566 |
| | no | | | |
| H32 | H21 | 2.57(8) | . | 2_566 |
| | no | | | |
| H42 | Cl19 | 2.90(4) | . | . |
| | no | | | |
| H61 | Pd1 | 3.68(4) | . | . |
| | no | | | |
| H61 | C131 | 3.04(4) | . | . |
| | no | | | |
| H61 | H501 | 2.37(6) | . | . |
| | no | | | |
| H61 | C501 | 2.69(4) | . | . |
| | no | | | |
| H62 | Pd2 | 3.66(5) | . | . |
| | no | | | |
| H62 | C502 | 2.79(5) | . | . |
| | no | | | |
| H62 | H502 | 2.33(8) | . | . |
| | no | | | |
| H81 | H401 | 2.38(8) | . | . |
| | no | | | |
| H81 | Pd1 | 3.02(3) | . | . |
| | no | | | |
| H81 | Cl1 | 2.39(9) | . | . |
| | no | | | |
| H82 | H402 | 2.48(8) | . | . |

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          no
H82       Cl2          2.42(9)                    .       .
          no
H82       Pd2          3.17(4)                    .       .
          no
H102      Cl11         3.12(6)                    .     2_666
          no
H111      H432         2.46(8)                    .     2_566
          no
H111      Cl4          2.89(7)                    .     2_666
          no
H111      Cl22         3.11(5)                    .     1_556
          no
H112      H431         2.44(9)                    .     2_566
          no
H112      Cl11         2.94(5)                    .     2_666
          no
H112      Cl3          2.97(7)                    .       .
          no
H121      C141         2.92(5)                    .       .
          no
H121      C21          3.08(4)                    .       .
          no
H121      C131         2.98(5)                    .       .
          no
H122      Cl3          3.04(4)                    .       .
          no
H122      C142         2.74(5)                    .       .
          no
H122      H142         2.60(6)                    .       .
          no
H122      C132         2.83(5)                    .       .
          no
H141      Cl9          2.97(4)                    .     2_666
          no
H141      C11          2.54(5)                    .       .
          no
H141      C61          2.77(4)                    .       .
          no
H142      Cl19         2.91(5)                    .       .
          no
H142      H122         2.60(6)                    .       .
          no
H142      C62          2.80(5)                    .       .
          no
H142      C12          2.55(6)                    .       .
          no
H152      Cl7          2.93(5)                    .     2_665
          no
H171      H191         2.28(4)                    .       .
          no
H171      C122         2.79(6)                    .     2_666
          no
H171      C112         2.95(6)                    .     2_666
          no
H171      Cl3          3.13(4)                    .     2_666
          no
H172      C111         3.06(6)                    .     2_666
          no
H172      H12           2.5930                    .       .
          no
H172      H192         2.29(4)                    .       .
          no
H172      Cl4          2.83(4)                    .       .
          no
H172      C121         2.82(6)                    .     2_666
          no
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|---|---|---|---|---|
| H191 | Cl3 | 2.60(7) | . | 2_666 |
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| H191 | H171 | 2.28(4) | . | . |
| | no | | | |
| H191 | C211 | 2.87(3) | . | . |
| | no | | | |
| H192 | C212 | 2.78(3) | . | . |
| | no | | | |
| H192 | H172 | 2.29(4) | . | . |
| | no | | | |
| H192 | Cl4 | 2.62(7) | . | . |
| | no | | | |
| H201 | H212 | 2.5729 | . | . |
| | no | | | |
| H201 | Cl2 | 2.8412 | . | . |
| | no | | | |
| H202 | H221 | 2.3149 | . | . |
| | no | | | |
| H202 | C221 | 3.0050 | . | . |
| | no | | | |
| H202 | C282 | 2.9486 | . | . |
| | no | | | |
| H203 | Cl4 | 2.5534 | . | . |
| | no | | | |
| H204 | C281 | 2.9167 | . | . |
| | no | | | |
| H204 | H281 | 2.5246 | . | . |
| | no | | | |
| H205 | Cl4 | 2.5645 | . | . |
| | no | | | |
| H205 | H272 | 2.4685 | . | . |
| | no | | | |
| H211 | C191 | 3.04(5) | . | . |
| | no | | | |
| H211 | Cl7 | 2.98(4) | . | 1_556 |
| | no | | | |
| H212 | C1 | 3.06(4) | . | . |
| | no | | | |
| H212 | H201 | 2.5729 | . | . |
| | no | | | |
| H212 | Cl6 | 2.73(4) | . | . |
| | no | | | |
| H212 | C192 | 2.95(5) | . | . |
| | no | | | |
| H221 | H202 | 2.3149 | . | 1_556 |
| | no | | | |
| H221 | C2 | 3.07(8) | . | 1_556 |
| | no | | | |
| H222 | Cl6 | 3.13(5) | . | . |
| | no | | | |
| H231 | Cl14 | 3.14(5) | . | 2_656 |
| | no | | | |
| H232 | Cl15 | 2.99(5) | . | . |
| | no | | | |
| H241 | Cl15 | 3.03(3) | . | . |
| | no | | | |
| H241 | C271 | 2.87(5) | . | . |
| | no | | | |
| H242 | Cl17 | 3.00(7) | . | . |
| | no | | | |
| H242 | C272 | 2.87(5) | . | . |
| | no | | | |
| H271 | C241 | 2.88(5) | . | . |
| | no | | | |
| H271 | Cl18 | 3.13(9) | . | . |
| | no | | | |
| H272 | C242 | 2.87(5) | . | . |

| | | | | | |
|---|---|---|---|---|---|
| | | no | | | |
| H272 | H205 | 2.4685 | . | . | |
| | | no | | | |
| H272 | C5 | 3.02(9) | . | . | |
| | | no | | | |
| H281 | Cl12 | 2.92(6) | . | . | |
| | | no | | | |
| H281 | H204 | 2.5246 | . | . | |
| | | no | | | |
| H291 | C341 | 2.80(7) | . | 2_556 | |
| | | no | | | |
| H291 | C371 | 3.01(7) | . | 2_556 | |
| | | no | | | |
| H291 | C331 | 2.93(6) | . | 2_556 | |
| | | no | | | |
| H291 | C381 | 3.05(6) | . | 2_556 | |
| | | no | | | |
| H291 | C361 | 2.91(8) | . | 2_556 | |
| | | no | | | |
| H291 | C351 | 2.80(8) | . | 2_556 | |
| | | no | | | |
| H292 | C352 | 2.90(8) | . | 2_555 | |
| | | no | | | |
| H292 | C342 | 2.93(7) | . | 2_555 | |
| | | no | | | |
| H301 | C501 | 2.95(6) | . | . | |
| | | no | | | |
| H301 | C321 | 2.86(4) | . | . | |
| | | no | | | |
| H302 | C502 | 2.95(6) | . | . | |
| | | no | | | |
| H302 | C322 | 2.86(5) | . | . | |
| | | no | | | |
| H310 | Cl3 | 3.1066 | . | . | |
| | | no | | | |
| H321 | C301 | 2.79(5) | . | . | |
| | | no | | | |
| H321 | H341 | 2.32(7) | . | . | |
| | | no | | | |
| H321 | C491 | 3.07(7) | . | 2_556 | |
| | | no | | | |
| H321 | C481 | 2.92(6) | . | 2_556 | |
| | | no | | | |
| H322 | C302 | 2.76(5) | . | . | |
| | | no | | | |
| H322 | C482 | 3.02(7) | . | 2_555 | |
| | | no | | | |
| H322 | H342 | 2.35(6) | . | . | |
| | | no | | | |
| H340 | Cl3 | 2.6774 | . | . | |
| | | no | | | |
| H341 | Cl2 | 2.90(5) | . | 2_556 | |
| | | no | | | |
| H341 | H321 | 2.32(7) | . | . | |
| | | no | | | |
| H341 | C491 | 3.06(3) | . | 2_556 | |
| | | no | | | |
| H342 | Cl1 | 2.87(5) | . | 2_556 | |
| | | no | | | |
| H342 | H322 | 2.35(6) | . | . | |
| | | no | | | |
| H351 | Cl2 | 2.81(7) | . | 2_556 | |
| | | no | | | |
| H352 | Cl1 | 2.82(7) | . | 2_556 | |
| | | no | | | |
| H352 | C241 | 3.07(6) | . | 2_556 | |
| | | no | | | |

| | | | | |
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| H360 | Cl3 | 2.8782 | . | . |
| | no | | | |
| H361 | Cl16 | 3.08(5) | . | 1_455 |
| | no | | | |
| H361 | C232 | 2.98(4) | . | 2_556 |
| | no | | | |
| H361 | C242 | 2.86(4) | . | 2_556 |
| | no | | | |
| H362 | C241 | 2.87(4) | . | 2_556 |
| | no | | | |
| H362 | C231 | 3.00(4) | . | 2_556 |
| | no | | | |
| H371 | C391 | 2.55(5) | . | . |
| | no | | | |
| H371 | C401 | 2.78(5) | . | . |
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| H372 | C392 | 2.48(5) | . | . |
| | no | | | |
| H372 | C5 | 3.09(4) | . | 1_455 |
| | no | | | |
| H372 | H15 | 2.2330 | . | 1_455 |
| | no | | | |
| H372 | C402 | 2.65(5) | . | . |
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| H401 | Cl1 | 2.68(5) | . | . |
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| H401 | Pd1 | 3.38(6) | . | . |
| | no | | | |
| H401 | C81 | 2.92(5) | . | . |
| | no | | | |
| H401 | H81 | 2.38(8) | . | . |
| | no | | | |
| H402 | H82 | 2.48(8) | . | . |
| | no | | | |
| H402 | Pd2 | 3.55(6) | . | . |
| | no | | | |
| H402 | C82 | 3.01(5) | . | . |
| | no | | | |
| H402 | Cl2 | 3.06(5) | . | . |
| | no | | | |
| H421 | Cl19 | 3.04(4) | . | 2_566 |
| | no | | | |
| H421 | Cl3 | 3.04(5) | . | 2_566 |
| | no | | | |
| H422 | Cl4 | 3.07(5) | . | 1_455 |
| | no | | | |
| H431 | H14 | 2.5580 | . | 1_455 |
| | no | | | |
| H431 | Cl11 | 2.97(4) | . | 1_455 |
| | no | | | |
| H431 | H112 | 2.44(9) | . | 2_566 |
| | no | | | |
| H431 | C112 | 2.95(5) | . | 2_566 |
| | no | | | |
| H432 | H111 | 2.46(8) | . | 2_566 |
| | no | | | |
| H441 | H461 | 2.49(5) | . | . |
| | no | | | |
| H441 | C451 | 2.76(3) | . | . |
| | no | | | |
| H441 | C461 | 2.62(5) | . | . |
| | no | | | |
| H442 | C462 | 2.70(5) | . | . |
| | no | | | |
| H442 | C452 | 2.71(3) | . | . |
| | no | | | |
| H461 | H441 | 2.49(5) | . | . |

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          no
 H461    C381        3.04(5)                    .       .
          no
 H461    C441        2.99(3)                    .       .
          no
 H462    C372        3.04(4)                    .       .
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 H462    C382        2.89(5)                    .       .
          no
 H462    Cl13        3.14(6)                    .     1_455
          no
 H472    Cl16        3.11(6)                    .     1_454
          no
 H481    C362        3.09(9)                    .       .
          no
 H482    C361        3.02(9)                    .       .
          no
 H491    Cl2         3.01(5)                    .       .
          no
 H492    Cl1         2.73(6)                    .       .
          no
 H501    H61         2.37(6)                    .       .
          no
 H501    Pd1         2.96(4)                    .       .
          no
 H502    Cl8         2.92(9)                    .       .
          no
 H502    C62         3.06(6)                    .       .
          no
 H502    Pd2         2.99(4)                    .       .
          no
 H502    H62         2.33(8)                    .       .
          no
 H620    Cl3          2.7044                    .     2_666
          no
 H620    C241         3.0796                    .       .
          no
 H630    C241         3.0207                    .       .
          no
 H630    Cl3          2.7381                    .     2_666
          no

loop_
_geom_bond_atom_site_label_D
_geom_bond_atom_site_label_H
_geom_contact_atom_site_label_A
_geom_bond_distance_DH
_geom_contact_distance_HA
_geom_contact_distance_DA
_geom_angle_DHA
_geom_contact_site_symmetry_A
#
#D   H   A   D - H  H...A   D...A    D - H...A  symm(A)
#
C2      H12     Cl4         0.9704     2.7395  3.613(11)
149.98     .
C4      H14     Cl3         0.9709     2.7903  3.682(10)
153.08   2_666
C81     H81     Cl1        0.99(9)    2.39(9)   3.371(8)
178(4)     .
C82     H82     Cl2        0.96(9)    2.42(9)   3.369(8)
168(5)     .
C172    H172    Cl4        0.98(6)    2.83(4)   3.660(8)
143(3)     .
C191    H191    Cl3        0.86(7)    2.60(7)   3.405(9)
155(3)   2_666
C192    H192    Cl4        0.94(7)    2.62(7)   3.368(9)
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137(3)     .
C3      H203    Cl4         0.9708     2.5534  3.472(12)
157.83     .
C5      H205    Cl4         0.9707     2.5645  3.507(18)
163.86     .
C212    H212    Cl6        0.92(6)    2.73(4)   3.468(8)
138(4)     .
C351    H351    Cl2        0.94(7)    2.81(7)   3.466(8)
128(4)   2_556
C352    H352    Cl1        0.87(7)    2.82(7)   3.411(8)
126(4)   2_556
C401    H401    Cl1        0.99(5)    2.68(5)   3.590(8)
154(3)     .
C492    H492    Cl1        0.87(6)    2.73(6)  3.565(10)
161(4)     .
C6      H620    Cl3         0.9698     2.7044  3.450(12)
134.06   2_666

# End of Crystallographic Information File

# Complex # 4

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;
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 Refinement on F^2^ for ALL reflections except for 186 with very
negative F^2^
 or flagged by the user for potential systematic errors.
Weighted R-factors
 wR and all goodnesses of fit S are based on F^2^, conventional
R-factors R
 are based on F, with F set to zero for negative F^2^. The
observed criterion
 of F^2^ > 2sigma(F^2^) is used only for calculating
_R_factor_obs etc. and is
 not relevant to the choice of reflections for refinement.
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R-factors based
 on F^2^ are statistically about twice as large as those based on
F, and R-
 factors based on ALL data will be even larger.
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Cl3 Cl 0.0651(5) 0.4351(5) 0.05016(11) 0.120(2) Uani 1 d . .
C16 C 0.3011(10) 0.3500(8) 0.0596(3) 0.041(2) Uani 1 d . .
H161 H 0.2595(10) 0.3445(8) 0.0334(3) 0.049 Uiso 1 calc R .
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H191 H 0.1366(8) 0.0521(8) 0.1267(3) 0.048 Uiso 1 calc R .
C26 C 0.4463(9) 0.2375(11) 0.3060(3) 0.049(3) Uani 1 d . .
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H121 H 0.7027(10) 0.5695(9) 0.2327(3) 0.070 Uiso 1 calc R .
C23 C 0.0800(9) -0.1600(9) 0.2632(3) 0.045(3) Uani 1 d . .
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C3 C 0.7766(10) 0.3047(12) 0.1778(3) 0.059(3) Uani 1 d . .
H31 H 0.7943(10) 0.2485(12) 0.1888(3) 0.071 Uiso 1 calc R .
C9 C 0.4436(14) 0.6143(11) 0.2482(3) 0.072(4) Uani 1 d . .
H91 H 0.3792(14) 0.6259(11) 0.2521(3) 0.087 Uiso 1 calc R .
C5 C 0.8305(11) 0.4787(11) 0.1356(3) 0.057(3) Uani 1 d . .
H51 H 0.8869(11) 0.5407(11) 0.1182(3) 0.069 Uiso 1 calc R .
C1 C 0.6431(8) 0.3862(9) 0.1751(3) 0.039(2) Uani 1 d . .
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H81 H 0.3583(12) 0.4657(10) 0.2125(3) 0.071 Uiso 1 calc R .
C4 C 0.8505(11) 0.3894(12) 0.1495(4) 0.060(3) Uani 1 d . .
H41 H 0.9169(11) 0.3878(12) 0.1389(4) 0.072 Uiso 1 calc R .
C21 C 0.2223(8) 0.0222(9) 0.2266(3) 0.036(2) Uani 1 d . .
C27 C 0.5262(10) 0.2463(12) 0.3451(3) 0.069(4) Uani 1 d . .
H271 H 0.6076(11) 0.2885(68) 0.3355(9) 0.103 Uiso 1 calc R .
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C10 C 0.5537(15) 0.6933(12) 0.2662(3) 0.073(4) Uani 1 d . .
H101 H 0.5623(15) 0.7584(12) 0.2824(3) 0.088 Uiso 1 calc R .
C11 C 0.6472(11) 0.6791(11) 0.2612(4) 0.063(3) Uani 1 d . .
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H291 H -0.0216(15) 0.5434(13) 0.0414(4) 0.127 Uiso 1 calc R .
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C28 C 0.1336(12) 0.2470(12) 0.2718(4) 0.075(4) Uani 1 d . .
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0.0147(13)
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C20 0.027(5) 0.025(5) 0.036(4) -0.003(4) 0.002(4) 0.012(5)
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C18 0.042(6) 0.032(6) 0.031(3) 0.005(4) 0.004(4) 0.020(5)
C7 0.056(7) 0.016(5) 0.045(4) 0.000(4) 0.006(4) 0.009(5)
C25 0.026(5) 0.022(5) 0.048(4) 0.000(4) 0.004(4) 0.012(4)
C22 0.045(6) 0.026(5) 0.032(4) 0.004(3) -0.003(4) 0.007(5)
C19 0.037(6) 0.036(6) 0.037(4) -0.006(4) 0.001(4) 0.021(5)
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C14 0.051(6) 0.023(5) 0.052(4) -0.002(4) 0.000(4) 0.012(5)
C12 0.057(7) 0.022(6) 0.059(5) -0.011(5) 0.010(5) -0.007(6)
C23 0.039(6) 0.045(6) 0.052(5) 0.012(4) 0.009(4) 0.021(5)
C17 0.044(7) 0.050(7) 0.038(4) 0.002(4) 0.002(4) 0.026(6)
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O2 0.074(6) 0.078(6) 0.040(3) -0.010(3) -0.005(3) 0.055(5)
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are taken
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distances, angles
 and torsion angles; correlations between esds in cell parameters
are only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
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l.s. planes.
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O1 Pd1 P1 100.0(2) . . ?
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#===============================================================
# Dr. A.L.Spek, Laboratory of Crystal and Structural Chemistry
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